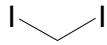
Property Data Sheet - Liquid Data Base **Rev. 1.0a** **Date: 01.12.1998**

Name: **Methylene Iodide**
IUPAC-Name: **Diiodomethane**

Sum formula: CH2I2
CAS-Ref.-No.: 75-11-6
Structure formula:



Beilstein-Ref.: E IV 1, p. 96
Merck-Index: 11,5985; 12,6143
Smiles Notation: C(I)I

Synonyms: Methylene diiodide; Dijodmethan; Methylenjodid; Mi-gee; Methyl diiodide

Property	Coeffic./Unit	Value	Notes/References
Molecular Weight	g/mol	267.836	based on IUPAC 1995 Atomic Weights: T.B. Coplen, J. Phys. Chem. Ref. Data 26 (1997), p. 1239
Critical Temperature	K	747.87	estim. rev. Lydersen method
		740.92	estim. Joback method
Critical Pressure	bar	47.32	estim. rev. Lydersen method
		54.23	estim. Joback method
Critical Volume	cm³/mol	252.3	estim. rev. Lydersen method
		267.5	estim. Joback method
Melting Point	K	279.25	CRC Hdb 97/98 #7506 [1]
	°C	6.1	CRC Hdb 97/98 #7506 [1]
Normal Boiling Point	K	455.2	CRC Hdb 97/98 #7506 [1]
	°C	182	CRC Hdb 97/98 #7506 [1]
Density	g/cm³	3.3254	@ 293 K, D'Ans-Lax, 1998, p.1017
		3.3212	@ 20 °C, CRC Hdb 97/98 #7506 [1]
		3.3079	@ 25 °C, Riddick et al. 1986 [5]
Density Function			d = A + BT + BT², T = temperature (°C)
d = Density (g/cm³)	A, g/cm³	3.3707 ± 0.0019	eval. regression with meas. data from A.I. Vogel et. al.,
Tmin (12 °C)	B, g/cm³/K	-2.4958E-3	J. Chem. Soc. 1948, p. 1850, V. Griffing et al., J. Phys.
Tmax (120 °C)	C, g/cm³/K²	-8.6689E-8	Chem. 58 (1954) p. 1054, Beilstein E III 1, p. 100
Molar Volume	cm³/mol	80.64	@ 20 °C, eval. from Density, CRC Hdb 97/98 #7506
Color/Odor	-	-	Light-yellow, clear liquid with a chloroform like odor, light-sensitive
Flash Point	°C	>112	Catalog Acros Organics
		104	Riddick et al. 1986 [5]
Vapor Pressure @ 20 °C	Torr	0.85	from Vapor Pressure Equation Parameters
Vapor Pressure Equation Parameters			log10(P) = A + BT + C log10(T) + DT², T = temp. (K)
P = Vapor pressure (bar)	A	39.5746	eval. Daubert et al., 1989 [6]
Tmin (279.25 K)	B, 1/K	-4052.75	eval. Daubert et al., 1989 [6]
Tmax (747.00 K)	C	-11.711	eval. Daubert et al., 1989 [6]
	D 1/K²	2.2058E-6	eval. Daubert et al., 1989 [6]
Acentric Factor	1	0.1468	eval. Lee-Kessler Equation Parameters
		0.1405	eval. Daubert et al., 1989 [6], Tc = 747.00 K
IG Enthalphy of Formation	kJ/mol	118.0 ± 4.2	meas. Kudchadker and Kudchadker, 1976 [8]
		90.0	estim. MOPAC 6.0, MNDO method (21.50 kcal/mol)
		90.0	estim. MOPAC 6.0, AM1 method (21.50 kcal/mol)
		89.8	estim. Joback method (21.44 kcal/mol)
Liq Enthalphy of Formation	kJ/mol	68.5 ± 0.8	meas. Carson, Laye, et al., 1993 [10]
Enthalphy of Fusion	kJ/mol	12.05	@ 279.25 K, Daubert et al., 1989 [6]
Enthalphy of Vaporization	kJ/mol	45.6	@ 298.15 K, meas. Carson, Laye, et al., 1994 [13]
		43.09	@ 298.15 K, estim. Watson method
		44.20	@ 298.15 K, estim. Pitzer method
		49.36	@ 298.15 K, eval. Daubert et al., 1989 [6]
Index of Refraction n[D,20]	-	1.7425	@ 20 °C, CRC Hdb 97/98 #7506 [1]
		1.74108	@ 20 °C, A.I. Vogel et. al., J. Chem. Soc. 1948, p. 1850
Molar Refraction: R[D,20]	cm³	32.57	@ 20 °C, eval. from n[D,20], CRC Hdb 97/98 #7506 [1]
Polarizability	Å³	12.90	CRC Hdb 97/98, p. 10-206
		13.00	estim. MOPAC 6.0, MNDO method
		12.42	estim. Group contributions method
Ionization Energy	eV	9.46 ± 0.02	meas. Tsai, Baer, et al., 1975 [14]
		10.87	estim. Hyperchem 5.02, MNDO method
		10.56	estim. Hyperchem 5.02, AM1 method

Property	Coeffic./Unit	Value	Notes/References
Constant Pressure Heat Capacity	J/(mol K)	133.81	@ 298.15 K, meas. Carson, Laye, et al., 1993 [10]
of liquid		112.8	@ 298.15 K, meas. Shehatta, 1993 [11]
		133.9	@ 298 K, meas. Kurbatov, 1948 [12]
Thermal Conductivity	W/(m K)	0.1015	@ 279.25 K, eval. Daubert et al., 1989 [6]
Viscosity	mPas	2.76 ± 0.05	@ 20 °C, eval. from regression, Yaws, 1995 [7]
Viscosity Function			$\log10(\eta) = A + B/T + CT + DT^2$, T = temperature (K)
η = Dynamic Viscosity (mPas)	A, 1	-1.461	Yaws, 1995 [7]
Tmin (279 K)	B, K	507.43	
Tmax (747 K)	C, 1/K	0.0011256	
	D, 1/K²	-1.847E-6	
Dielectric Constant (Permittivity)	1	5.32	@ 298.2 K, CRC Hdb 97/98, p. 6-141
		5.316	@ 25 °C, Riddick et al. 1986 [5]
Relative Permittivity Function			$\varepsilon = A + BT + CT^2 + DT^3$, T = temperature (°C)
ε = Permittivity (1)	A, 1	-	
Tmin (°C)	B, 1/K	-	
Tmax (°C)	C, 1/K²	-	
	D, 1/K³	-	
Dipole Moment:	D	1.08	@ 10..70 °C, meas. in Benzene, D'Ans-Lax [4], p. 3-303
		1.14	meas. in Hexane, Beilstein E III 1, p. 100
		1.10	meas. in Benzene, Beilstein E III 1, p. 100
		1.16	estim. Hyperchem 5.02, MNDO method
		1.13	estim. Hyperchem 5.02, AM1 method
Surface Tension	mN/m	50.88	@ 20 °C, G. Körösi et al., J. Chem. Eng. Data 26 (1981) p. 323
		50.0	H.J. Busscher et al., Coll. Surf. 9 (1984), p. 319-331
		50.8	F.M. Fowkes, Ind. Eng. Chem. 56 (1964) p. 48
		50.8	D.K.Owens et al., J. Appl. Polym. Sci. 13 (1969), p.1741
		50.8	G. Ström et al., J. Colloid Interf. Sci. 119 (1987), p. 352
Surface Tension Function			$\gamma = A + BT + CT^2$, T = temperature (°C)
γ = Surface Tension (mN/m)	A, mN/m	53.48 ± 0.07	from regression, LB IV/16, 1961-98 [3], p. 144
Tmin (0 °C)	B, mN/m/K	-0.14154	
Tmax (100 °C)	C, mN/m/K²	4.9567E-5	
Dispersion Force Contribution	mN/m	47.4	H.J. Busscher et al, Coll. Surf. 9 (1984), p. 319-331
of Surface Tension @ 20 °C		48.5 ± 9	F.M. Fowkes, Ind. Eng. Chem. 56 (1964) p. 48
		49.5 ± 1	D.K.Owens et al., J. Appl. Polym. Sci. 13 (1969), p.1741
		50.8	G. Ström et al., J. Colloid Interf. Sci. 119 (1987), p. 352
Polar Force Contribution	mN/m	2.6	H.J. Busscher et al, Coll. Surf. 9 (1984), p. 319-331
of Surface Tension @ 20 °C		2.3	F.M. Fowkes, Ind. Eng. Chem. 56 (1964) p. 48
		1.3	D.K.Owens et al., J. Appl. Polym. Sci. 13 (1969), p.1741
		0.0	G. Ström et al., J. Colloid Interf. Sci. 119 (1987), p. 352
Acid-Base (A-B) Contributions	total, mN/m	50.8	M.L. Gonzalez-Martin et al., Langmuir 13 (1997), p. 5991
of Surface Tension	LW, mN/m	50.8	
	A, mN/m	0.72	
	B, mN/m	0.00	
Parachor	1	215.0	eval. from meas. Surface Tension and Density, CRC Hdb 97/98 #7506 [1]
Interfacial Tension vs. water	mN/m	35.86 ± 0.37	@ 20 °C, DataPhysics Instruments GmbH, 1998
		41.6	W. Fox: J. Am. Chem. Soc. 67 (1945) p. 700, E.G. Carter, D.C. Jones, Trans. Faraday Soc. 30 (1934) p. 1027
		48.50	@ 20 °C, W.D. Harkins, A. Feldmann, J. Am. Chem. Soc. 44 (1922) 2665 (2673)
Interfacial Tension vs. water Function			$\gamma_{ow} = A + BT$, T = temperature (°C)
γ_{ow} = Interfacial Tension (mN/m)	A, mN/m	38.04 ± 0.37	DataPhysics Instruments GmbH, 1998
Tmin (10 °C), Tmax (30 °C)	B, mN/m/K	-0.1085 ± 0.018	DataPhysics Instruments GmbH, 1998
Solubility in water	Mass-%	0.124	@ 30 °C, CRC Hdb 97/98, p. 8-87
Solubility of water	Mass-%	-	
Henry' Law Constant (water)	mol/kg bar	2.3	@ 298.15 K, Moore, Geen, et al., 1995 [19]
		2.8	@ 298.15 K, Yaws and Yang, 1992 [20]
	kPa m³/mol	0.032	@ 25 °C, CRC Hdb 97/98, p. 8-87 [1]
$d(\ln(k°_H))/d(1/T)$	K	5000	@ 298.15 K, Moore, Geen, et al., 1995 [19]

Property	Coeffic./Unit	Value	Notes/References
log P		2.30	meas. Pomona, 1987
		2.35	estim. LOGKOW, http://esc.syrres.com/~esc1/kowint.htm
		2.19	estim. Physical Properties Pro 2.0, group contrib.
		2.31	estim. CLOGP, http://www.daylight.com/daycgi/clogp
Hansen's 3D-Solubility Parameter			
total, @ 25 °C	MPa^(1/2)	19.0	CRC Hdb SCS, 1997, p. 331 [17]
dispersion	MPa^(1/2)	17.8	CRC Hdb SCS, 1997, p. 331 [17]
polar	MPa^(1/2)	3.9	CRC Hdb SCS, 1997, p. 331 [17]
H-bonding	MPa^(1/2)	5.5	CRC Hdb SCS, 1997, p. 331 [17]
Van der Waals Volume	cm³/mol	51.25	estim. Physical Properties Pro 2.0, MOLY geometry
		50.93	Daubert et al. 1989 [6]
Van der Waals Area	10^9 cm²/mol	6.903	estim. Physical Properties Pro 2.0, MOLY geometry
		6.430	Daubert et al. 1989 [6]

Structure

Molecular Structure (theor. calc., Hyperchem 5.02, AM1 method)
content of matrix:
column 1: element abbreviation, column 2: bond length in Å, column 3: vary? Y=1/N=0, column 4: bond angle in °,
column 5: vary? Y=1/N=0, column 6: dihedral angle in °, column 6: vary? Y=1/N=0, column 7: bond with atom #,
column 8: bond angle with atom # in column 7 and 8, column 9: dihedral angle with atom # in column 7, 8, and 9

AM1 UHF PRECISE GNORM=0.03
Name: D:\MOPAC6.0\Diiodmethane.mop
Sum formula: CH2I2

C	00000.0000	0	00000.0000	0	00000.0000	0	0	0	0
H	00001.1077	1	00000.0000	0	00000.0000	0	1	0	0
H	00001.1077	1	00109.3146	1	00000.0000	0	1	2	0
I	00002.0418	1	00108.7105	1	00241.4761	1	1	2	3
I	00002.0417	1	00108.7161	1	00118.5339	1	1	2	3

0

Additional References:

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