Methane, diiodo-

Other names:	CH2I2
	Diiodomethane
	Dijodmethan
	METHYL DIIODIDE
	METHYLENE IODIDE
	MI-Gee
	Methylene diiodide
	Methylenjodid
	Mi-gee brand
	NSC 35804
Inchi:	InChI=1S/CH2I2/c2-1-3/h1H2
InchiKey:	NZZFYRREKKOMAT-UHFFFAOYSA-N
Formula:	CH2I2
SMILES:	ICI
Mol. weight [g/mol]:	267.84
CAS:	75-11-6

Physical Properties

Property code	Value	Unit	Source
af	0.1800		KDB
chl	-747.80 ± 0.60	kJ/mol	NIST Webbook
gf	73.78	kJ/mol	Joback Method
hf	118.00 ± 4.20	kJ/mol	NIST Webbook
hf	122.00 ± 4.20	kJ/mol	NIST Webbook
hfl	68.50 ± 0.80	kJ/mol	NIST Webbook
hfus	7.16	kJ/mol	Joback Method
hvap	45.60	kJ/mol	NIST Webbook
hvap	49.00	kJ/mol	NIST Webbook
hvap	45.60	kJ/mol	NIST Webbook
ie	9.46 ± 0.02	eV	NIST Webbook
ie	9.46 ± 0.02	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
log10ws	-2.34		Aqueous Solubility Prediction Method
log10ws	-2.34		Estimated Solubility Method

logp	1.814		Crippen Method
mcvol	76.590	ml/mol	McGowan Method
pc	5420.00	kPa	KDB
rinpol	911.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	878.00		NIST Webbook
ripol	1510.47		NIST Webbook
ripol	1522.18		NIST Webbook
tb	455.20	K	KDB
tc	740.90	K	KDB
tf	278.93	K	Aqueous Solubility Prediction Method
tf	279.00	K	KDB
vc	0.268	m3/kmol	KDB
zc	0.2353570		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	81.08	J/mol×K	665.08	Joback Method
cpg	73.16	J/mol×K	451.31	Joback Method
cpg	70.80	J/mol×K	408.56	Joback Method
cpg	79.89	J/mol×K	622.32	Joback Method
cpg	78.54	J/mol×K	579.57	Joback Method
cpg	76.99	J/mol×K	536.82	Joback Method
cpg	75.21	J/mol×K	494.07	Joback Method
cpl	112.80	J/mol×K	298.15	NIST Webbook
cpl	133.90	J/mol×K	298.00	NIST Webbook
cpl	133.81	J/mol×K	298.15	NIST Webbook
dvisc	0.0005376	Pa×s	408.56	Joback Method
dvisc	0.0018577	Pa×s	280.95	Joback Method
dvisc	0.0030891	Pa×s	249.05	Joback Method
dvisc	0.0059647	Pa×s	217.15	Joback Method
dvisc	0.0006774	Pa×s	376.66	Joback Method
dvisc	0.0008910	Pa×s	344.76	Joback Method
dvisc	0.0012392	Pa×s	312.86	Joback Method
hfust	12.05	kJ/mol	279.20	NIST Webbook
hfust	12.10	kJ/mol	279.20	NIST Webbook
hvapt	45.40	kJ/mol	430.50	NIST Webbook

hvapt	48.80	kJ/mol	374.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40015e+01
Coeff. B	-3.62073e+03
Coeff. C	-6.82730e+01
Temperature range (K), min.	332.29
Temperature range (K), max.	486.28

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.24639e+01
Coeff. B	-9.19799e+03
Coeff. C	-1.12077e+01
Coeff. D	4.65037e-06
Temperature range (K), min.	279.25
Temperature range (K), max.	747.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75116&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1528
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
KDB: https://www.cheric.org/files/research/kdb/mol/mol1528.mol

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility