Benzene, 1,2-dichloro-3-methoxy-

Other names: 1,2-Dichloro-3-methoxybenzene
2,3-Dichloroanisole
Inchi: InChI=1S/C7H6Cl2O/c1-10-6-4-2-3-5(8)7(6)9/h2-4H,1H3
InchiKey: HFEASCCDHUVYKU-UHFFFAOYSA-N
Formula: C7H6Cl2O
SMILES: COc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 177.03
CAS: 1984-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-27.65	kJ/mol	Joback Method
hf	-137.92	kJ/mol	Joback Method
hfus	16.73	kJ/mol	Joback Method
hsub	83.60 ± 1.50	kJ/mol	NIST Webbook
hvap	45.96	kJ/mol	Joback Method
log10ws	-3.31		Aqueous Solubility Prediction Method
logp	3.002		Crippen Method
mcvol	116.080	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1336.80		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1336.80		NIST Webbook
rinpol	1306.00		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	1951.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1957.00		NIST Webbook

ripol	1977.00		NIST Webbook
tb	493.48	K	Joback Method
tc	720.45	K	Joback Method
tf	304.82	K	Aqueous Solubility Prediction Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.95	J/mol×K	493.48	Joback Method
cpg	216.08	J/mol×K	531.31	Joback Method
cpg	224.74	J/mol×K	569.14	Joback Method
cpg	232.93	J/mol×K	606.96	Joback Method
cpg	240.65	J/mol×K	644.79	Joback Method
cpg	247.90	J/mol×K	682.62	Joback Method
cpg	254.69	J/mol×K	720.45	Joback Method
dvisc	0.0013457	Pa×s	302.18	Joback Method
dvisc	0.0008743	Pa×s	334.06	Joback Method
dvisc	0.0006124	Pa×s	365.95	Joback Method
dvisc	0.0004541	Pa×s	397.83	Joback Method
dvisc	0.0003521	Pa×s	429.71	Joback Method
dvisc	0.0002827	Pa×s	461.60	Joback Method
dvisc	0.0002335	Pa×s	493.48	Joback Method
hfust	22.04	kJ/mol	304.10	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1984594&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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