Benzene, 1,2,3-trichloro-4-methoxy-

Other names: 2,3,4-Trichloroanisole
Inchi: InChI=1S/C7H5Cl3O/c1-11-5-3-2-4(8)6(9)7(5)10/h2-3H,1H3
InchiKey: FRQUNVLMWIYOLV-UHFFFAOYSA-N
Formula: C7H5Cl3O
SMILES: COc1ccc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 211.47
CAS: 54135-80-7

Physical Properties

Property code	Value	Unit	Source
gf	-49.21	kJ/mol	Joback Method
hf	-165.13	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	51.00	kJ/mol	Joback Method
log10ws	-4.29		Aqueous Solubility Prediction Method
logp	3.655		Crippen Method
mcvol	128.320	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1488.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2183.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2212.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2202.00		NIST Webbook
ripol	2212.00		NIST Webbook
ripol	2182.00		NIST Webbook

ripol	2183.00		NIST Webbook
ripol	2183.00		NIST Webbook
tb	535.89	K	Joback Method
tc	769.13	K	Joback Method
tf	342.65	K	Aqueous Solubility Prediction Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.05	J/mol×K	535.89	Joback Method
cpg	235.28	J/mol×K	574.76	Joback Method
cpg	243.06	J/mol×K	613.64	Joback Method
cpg	250.41	J/mol×K	652.51	Joback Method
cpg	257.31	J/mol×K	691.39	Joback Method
cpg	263.76	J/mol×K	730.26	Joback Method
cpg	269.77	J/mol×K	769.13	Joback Method
dvisc	0.0010690	Pa×s	344.62	Joback Method
dvisc	0.0007421	Pa×s	376.50	Joback Method
dvisc	0.0005454	Pa×s	408.38	Joback Method
dvisc	0.0004192	Pa×s	440.26	Joback Method
dvisc	0.0003338	Pa×s	472.13	Joback Method
dvisc	0.0002735	Pa×s	504.01	Joback Method
dvisc	0.0002296	Pa×s	535.89	Joback Method

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=C54135807&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
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