Benzene, 1,3,5-trichloro-2-methoxy-

Other names:	1,3,5-Trichloro-2-methoxybenzene
	2,4,6-Trichloroanisole
	Anisole, 2,4,6-trichloro-
	Methyl 2,4,6-trichlorophenyl ether
	Tyrene
Inchi:	InChI=1S/C7H5Cl3O/c1-11-7-5(9)2-4(8)3-6(7)10/h2-3H,1H3
InchiKey:	WCVOGSZTONGSQY-UHFFFAOYSA-N
Formula:	C7H5Cl3O
SMILES:	COc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	211.47
CAS:	87-40-1

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	-4.20		Aqueous Solubility Prediction Method
logp	3.655		Crippen Method
mcvol	128.320	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1350.80		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1350.00		NIST Webbook

rinpol	1327.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1350.80		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1302.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	535.89	K	Joback Method
tc	769.13	K	Joback Method
tf	334.40	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	263.76	J/mol×K	730.26	Joback Method
cpg	257.31	J/mol×K	691.39	Joback Method
cpg	250.41	J/mol×K	652.51	Joback Method
cpg	243.06	J/mol×K	613.64	Joback Method
cpg	235.28	J/mol×K	574.76	Joback Method
cpg	269.77	J/mol×K	769.13	Joback Method
dvisc	0.0002296	Pa×s	535.89	Joback Method
dvisc	0.0002735	Pa×s	504.01	Joback Method
dvisc	0.0003338	Pa×s	472.13	Joback Method
dvisc	0.0004192	Pa×s	440.26	Joback Method
dvisc	0.0005454	Pa×s	408.38	Joback Method
dvisc	0.0007421	Pa×s	376.50	Joback Method

dvisc	0.0010690	Pa×s	344.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	3.70	NIST Webbook
tbrp	513.20	K	98.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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=C87401&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume