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

Other names: 3,4,5-Trichloroanisole
Inchi: InChI=1S/C7H5Cl3O/c1-11-4-2-5(8)7(10)6(9)3-4/h2-3H,1H3
InchiKey: GUCFBWGWRCILHN-UHFFFAOYSA-N
Formula: C7H5Cl3O
SMILES: COc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]: 211.47
CAS: 54135-82-9

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	-3.65		Crippen Method
logp	3.655		Crippen Method
mcvol	128.320	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1437.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1431.00		NIST Webbook
ripol	2062.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2042.00		NIST Webbook
tb	535.89	K	Joback Method
tc	769.13	K	Joback Method
tf	344.62	K	Joback 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54135829&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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