2,3,6-TRICHLOROANISOLE

Other names: 2,3,6-Trichloroanisole
1,2,4-Trichloro-3-methoxybenzene
Inchi: InChI=1S/C7H5Cl3O/c1-11-7-5(9)3-2-4(8)6(7)10/h2-3H,1H3
InchiKey: OTFNCXLUCRUNCH-UHFFFAOYSA-N
Formula: C7H5Cl3O
SMILES: COc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 211.48

Physical Properties

Property code	Value	Unit	Source
hf	-146.34	kJ/mol	Cheméo Relay (1.0)
hfus	20.54	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	3.655		Crippen Method
mcvol	128.320	ml/mol	McGowan Method
rinpol	1350.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1393.70		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1358.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook

ripol	1909.00		NIST Webbook
tb	514.12	K	Cheméo Relay (1.0)
tf	310.38	K	Cheméo Relay (1.0)

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50375105&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point