2-METHOXY-3,6-DICHLORO-PHENOL

Inchi: InChI=1S/C7H6Cl2O2/c1-11-7-5(9)3-2-4(8)6(7)10/h2-3,10H,1H3
InchiKey: OBRQSFBOZCMSTK-UHFFFAOYSA-N
Formula: C7H6Cl2O2
SMILES: COc1c(Cl)ccc(Cl)c1O
Mol. weight [g/mol]: 193.03

Physical Properties

Property code	Value	Unit	Source
hf	-288.34	kJ/mol	Cheméo Relay (1.0)
hfus	22.51	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-2.41		Cheméo Relay (1.0)
logp	2.708		Crippen Method
mcvol	121.950	ml/mol	McGowan Method
tb	507.05	K	Cheméo Relay (1.0)
tf	343.00 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.37	J/mol×K	574.10	Joback Method
cpg	254.56	J/mol×K	613.96	Joback Method
cpg	262.19	J/mol×K	653.82	Joback Method
cpg	269.33	J/mol×K	693.68	Joback Method
cpg	276.01	J/mol×K	733.55	Joback Method
cpg	282.31	J/mol×K	773.41	Joback Method
cpg	288.27	J/mol×K	813.27	Joback Method
dvisc	0.0006281	Pa×s	413.90	Joback Method
dvisc	0.0003560	Pa×s	440.60	Joback Method
dvisc	0.0002153	Pa×s	467.30	Joback Method
dvisc	0.0001375	Pa×s	494.00	Joback Method
dvisc	0.0000919	Pa×s	520.70	Joback Method
dvisc	0.0000639	Pa×s	547.40	Joback Method

dvisc	0.0000460	Pa×s	574.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77102933&Units=SI
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):	

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point