2,3,4-trichloro-6-methoxyphenol

Inchi: InChI=1S/C7H5Cl3O2/c1-12-4-2-3(8)5(9)6(10)7(4)11/h2,11H,1H3
InchiKey: NIAJPNQTKGWEOI-UHFFFAOYSA-N
Formula: C7H5Cl3O2
SMILES: COc1cc(Cl)c(Cl)c(Cl)c1O
Mol. weight [g/mol]: 227.47

Physical Properties

Property code	Value	Unit	Source
gf	-203.83	kJ/mol	Joback Method
hf	-342.44	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.66		Aqueous Solubility Prediction Method
logp	3.361		Crippen Method
mcvol	134.190	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	616.51	K	Joback Method
tc	860.21	K	Joback Method
tf	456.34	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.76	J/mol×K	616.51	Joback Method
cpg	295.76	J/mol×K	819.59	Joback Method
cpg	290.08	J/mol×K	778.98	Joback Method
cpg	284.10	J/mol×K	738.36	Joback Method
cpg	277.75	J/mol×K	697.74	Joback Method
cpg	270.99	J/mol×K	657.13	Joback Method
cpg	301.17	J/mol×K	860.21	Joback Method
dvisc	0.0000339	Pa×s	616.51	Joback Method
dvisc	0.0000454	Pa×s	589.82	Joback Method

dvisc	0.0000626	Pa×s	563.12	Joback Method
dvisc	0.0000892	Pa×s	536.42	Joback Method
dvisc	0.0001318	Pa×s	509.73	Joback Method
dvisc	0.0002033	Pa×s	483.04	Joback Method
dvisc	0.0003298	Pa×s	456.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume