

3,4,5-Trichloro-2,6-dimethoxyphenol

Inchi:	InChI=1S/C8H7Cl3O3/c1-13-7-4(10)3(9)5(11)8(14-2)6(7)12/h12H,1-2H3
InchiKey:	ZZCSBXFJFLSDRR-UHFFFAOYSA-N
Formula:	C8H7Cl3O3
SMILES:	COc1c(O)c(OC)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	257.50

Physical Properties

Property code	Value	Unit	Source
gf	-310.04	kJ/mol	Joback Method
hf	-506.77	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-3.41		Aqueous Solubility Prediction Method
logp	3.370		Crippen Method
mcvol	154.150	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
tb	666.79	K	Joback Method
tc	902.60	K	Joback Method
tf	502.36	K	Joback Method
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.94	J/molxK	666.79	Joback Method
cpg	336.21	J/molxK	706.09	Joback Method
cpg	344.03	J/molxK	745.39	Joback Method
cpg	351.44	J/molxK	784.70	Joback Method
cpg	358.45	J/molxK	824.00	Joback Method
cpg	365.09	J/molxK	863.30	Joback Method
cpg	371.38	J/molxK	902.60	Joback Method
dvisc	0.0001422	Paxs	502.36	Joback Method
dvisc	0.0000926	Paxs	529.76	Joback Method

dvisc	0.0000629	Paxs	557.17	Joback Method
dvisc	0.0000443	Paxs	584.58	Joback Method
dvisc	0.0000322	Paxs	611.98	Joback Method
dvisc	0.0000241	Paxs	639.38	Joback Method
dvisc	0.0000184	Paxs	666.79	Joback Method

Sources

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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