(2,3,6-Trichlorophenoxy)acetic acid

Inchi: InChI=1S/C8H5Cl3O3/c9-4-1-2-5(10)8(7(4)11)14-3-6(12)13/h1-2H,3H2,(H,12,13)
InchiKey: GQOHYQAHKDLXCV-UHFFFAOYSA-N
Formula: C8H5Cl3O3
SMILES: O=C(O)COc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 255.48
CAS: 4007-00-5

Physical Properties

Property code	Value	Unit	Source
gf	-306.53	kJ/mol	Joback Method
hf	-450.58	kJ/mol	Joback Method
hfus	28.82	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.110		Crippen Method
mcvol	149.850	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	704.82	K	Joback Method
tc	922.43	K	Joback Method
tf	466.64	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.10	J/mol×K	704.82	Joback Method
cpg	343.26	J/mol×K	886.16	Joback Method
cpg	338.40	J/mol×K	849.89	Joback Method
cpg	333.05	J/mol×K	813.63	Joback Method
cpg	327.22	J/mol×K	777.36	Joback Method
cpg	320.91	J/mol×K	741.09	Joback Method
cpg	347.64	J/mol×K	922.43	Joback Method
dvisc	0.0000544	Pa×s	704.82	Joback Method
dvisc	0.0000735	Pa×s	665.12	Joback Method

dvisc	0.0001030	Pa×s	625.43	Joback Method
dvisc	0.0001513	Pa×s	585.73	Joback Method
dvisc	0.0002349	Pa×s	546.03	Joback Method
dvisc	0.0003908	Pa×s	506.34	Joback Method
dvisc	0.0007091	Pa×s	466.64	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4007005&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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