2,4,5-Trichlorophenyl salicylate

Inchi: InChI=1S/C13H7Cl3O3/c14-8-5-10(16)12(6-9(8)15)19-13(18)7-3-1-2-4-11(7)17/h1-6,17H
InchiKey: UGFUAUFSBFLNLL-UHFFFAOYSA-N
Formula: C13H7Cl3O3
SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccccc1O
Mol. weight [g/mol]: 317.55

Physical Properties

Property code	Value	Unit	Source
gf	-169.82	kJ/mol	Joback Method
hf	-342.33	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	86.39	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.572		Crippen Method
mcvol	196.540	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	834.34	K	Joback Method
tc	1097.03	K	Joback Method
tf	600.31	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.23	J/mol×K	834.34	Joback Method
cpg	507.40	J/mol×K	1053.25	Joback Method
cpg	500.19	J/mol×K	1009.47	Joback Method
cpg	492.67	J/mol×K	965.69	Joback Method
cpg	484.74	J/mol×K	921.90	Joback Method
cpg	476.30	J/mol×K	878.12	Joback Method
cpg	514.43	J/mol×K	1097.03	Joback Method
dvisc	0.0000070	Pa×s	834.34	Joback Method
dvisc	0.0000093	Pa×s	795.34	Joback Method
dvisc	0.0000127	Pa×s	756.33	Joback Method

dvisc	0.0000180	Pa×s	717.33	Joback Method
dvisc	0.0000266	Pa×s	678.32	Joback Method
dvisc	0.0000411	Pa×s	639.32	Joback Method
dvisc	0.0000673	Pa×s	600.31	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=B6004192&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