2,3,4,6-Tetrachlorophenyl salicylate

Inchi: InChI=1S/C13H6Cl4O3/c14-7-5-8(15)12(11(17)10(7)16)20-13(19)6-3-1-2-4-9(6)18/h1-5,1
InchiKey: OAZWQPUQRAFSIK-UHFFFAOYSA-N
Formula: C13H6Cl4O3
SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccccc1O
Mol. weight [g/mol]: 352.00
CAS: 116465-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-191.38	kJ/mol	Joback Method
hf	-369.54	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.225		Crippen Method
mcvol	208.780	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	876.75	K	Joback Method
tc	1141.39	K	Joback Method
tf	642.75	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.15	J/mol×K	876.75	Joback Method
cpg	518.98	J/mol×K	1097.28	Joback Method
cpg	512.24	J/mol×K	1053.18	Joback Method
cpg	505.29	J/mol×K	1009.07	Joback Method
cpg	498.02	J/mol×K	964.96	Joback Method
cpg	490.34	J/mol×K	920.86	Joback Method
cpg	525.62	J/mol×K	1141.39	Joback Method
dvisc	0.0000055	Pa×s	876.75	Joback Method
dvisc	0.0000072	Pa×s	837.75	Joback Method

dvisc	0.0000096	Pa×s	798.75	Joback Method
dvisc	0.0000132	Pa×s	759.75	Joback Method
dvisc	0.0000187	Pa×s	720.75	Joback Method
dvisc	0.0000278	Pa×s	681.75	Joback Method
dvisc	0.0000432	Pa×s	642.75	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C116465500&Units=SI

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