

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/molxK	834.34	Joback Method
cpg	507.40	J/molxK	1053.25	Joback Method
cpg	500.19	J/molxK	1009.47	Joback Method
cpg	492.67	J/molxK	965.69	Joback Method
cpg	484.74	J/molxK	921.90	Joback Method
cpg	476.30	J/molxK	878.12	Joback Method
cpg	514.43	J/molxK	1097.03	Joback Method
dvisc	0.0000070	Paxs	834.34	Joback Method
dvisc	0.0000093	Paxs	795.34	Joback Method
dvisc	0.0000127	Paxs	756.33	Joback Method

dvisc	0.0000180	Paxs	717.33	Joback Method
dvisc	0.0000266	Paxs	678.32	Joback Method
dvisc	0.0000411	Paxs	639.32	Joback Method
dvisc	0.0000673	Paxs	600.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004192&Units=SI
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

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
hvac:	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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