

Pentachlorophenyl salicylate

Inchi:	InChI=1S/C13H5Cl5O3/c14-7-8(15)10(17)12(11(18)9(7)16)21-13(20)5-3-1-2-4-6(5)19/h1
InchiKey:	ZMZPNTFEPFRJHW-UHFFFAOYSA-N
Formula:	C13H5Cl5O3
SMILES:	O=C(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)c1ccccc1O
Mol. weight [g/mol]:	386.44
CAS:	36994-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-212.94	kJ/mol	Joback Method
hf	-396.75	kJ/mol	Joback Method
hfus	45.12	kJ/mol	Joback Method
hvap	96.49	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.878		Crippen Method
mcvol	221.020	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	919.16	K	Joback Method
tc	1185.72	K	Joback Method
tf	685.19	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.84	J/molxK	919.16	Joback Method
cpg	503.28	J/molxK	963.59	Joback Method
cpg	510.29	J/molxK	1008.01	Joback Method
cpg	516.98	J/molxK	1052.44	Joback Method
cpg	523.44	J/molxK	1096.87	Joback Method
cpg	529.77	J/molxK	1141.29	Joback Method
cpg	536.06	J/molxK	1185.72	Joback Method
dvisc	0.0000287	Paxs	685.19	Joback Method
dvisc	0.0000192	Paxs	724.19	Joback Method

dvisc	0.0000134	Paxs	763.18	Joback Method
dvisc	0.0000097	Paxs	802.17	Joback Method
dvisc	0.0000072	Paxs	841.17	Joback Method
dvisc	0.0000055	Paxs	880.16	Joback Method
dvisc	0.0000043	Paxs	919.16	Joback Method

Sources

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=C36994691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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