Pentachlorophenol, isoBOC

Inchi: InChI=1S/C11H9Cl5O3/c1-4(2)3-18-11(17)19-10-8(15)6(13)5(12)7(14)9(10)16/h4H,3H2,
InchiKey: HHZUPNNIJGBWFU-UHFFFAOYSA-N
Formula: C11H9Cl5O3
SMILES: CC(C)COC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
gf	-295.01	kJ/mol	Joback Method
hf	-552.19	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	78.77	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	6.125		Crippen Method
mcvol	216.600	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	788.08	K	Joback Method
tc	1019.40	K	Joback Method
tf	531.74	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.25	J/mol×K	788.08	Joback Method
cpg	490.32	J/mol×K	826.63	Joback Method
cpg	498.59	J/mol×K	865.19	Joback Method
cpg	506.06	J/mol×K	903.74	Joback Method
cpg	512.68	J/mol×K	942.29	Joback Method
cpg	518.46	J/mol×K	980.85	Joback Method
cpg	523.37	J/mol×K	1019.40	Joback Method
dvisc	0.0004302	Pa×s	531.74	Joback Method

dvisc	0.0003029	Pa×s	574.46	Joback Method
dvisc	0.0002239	Pa×s	617.19	Joback Method
dvisc	0.0001721	Pa×s	659.91	Joback Method
dvisc	0.0001366	Pa×s	702.63	Joback Method
dvisc	0.0001113	Pa×s	745.36	Joback Method
dvisc	0.0000928	Pa×s	788.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235331&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume