Pentachlorophenol, O-trifluoroacetyl-

Inchi: InChI=1S/C8Cl5F3O2/c9-1-2(10)4(12)6(5(13)3(1)11)18-7(17)8(14,15)16
InchiKey: QACUOWCDCMROJT-UHFFFAOYSA-N
Formula: C8Cl5F3O2
SMILES: O=C(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)C(F)(F)F
Mol. weight [g/mol]: 362.35

Physical Properties

Property code	Value	Unit	Source
gf	-794.42	kJ/mol	Joback Method
hf	-949.85	kJ/mol	Joback Method
hfus	34.17	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.421		Crippen Method
mcvol	173.770	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	692.04	K	Joback Method
tc	917.09	K	Joback Method
tf	494.89	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.56	J/mol×K	692.04	Joback Method
cpg	344.08	J/mol×K	729.55	Joback Method
cpg	349.09	J/mol×K	767.06	Joback Method
cpg	353.60	J/mol×K	804.56	Joback Method
cpg	357.65	J/mol×K	842.07	Joback Method
cpg	361.24	J/mol×K	879.58	Joback Method
cpg	364.39	J/mol×K	917.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374848&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
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