2,3,5-Trichlorophenol, O-pentafluoropropionyl-

Inchi: InChI=1S/C9H2Cl3F5O2/c10-3-1-4(11)6(12)5(2-3)19-7(18)8(13,14)9(15,16)17/h1-2H
InchiKey: PULPAWQMCVAFSA-UHFFFAOYSA-N
Formula: C9H2Cl3F5O2
SMILES: O=C(Oc1cc(Cl)cc(Cl)c1Cl)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 343.46

Physical Properties

Property code	Value	Unit	Source
gf	-1129.66	kJ/mol	Joback Method
hf	-1317.04	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.750		Crippen Method
mcvol	166.920	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1284.00		NIST Webbook
rinpol	1284.00		NIST Webbook
tb	625.41	K	Joback Method
tc	831.17	K	Joback Method
tf	424.88	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.87	J/mol×K	625.41	Joback Method
cpg	379.66	J/mol×K	659.70	Joback Method
cpg	386.75	J/mol×K	694.00	Joback Method
cpg	393.21	J/mol×K	728.29	Joback Method
cpg	399.06	J/mol×K	762.59	Joback Method
cpg	404.35	J/mol×K	796.88	Joback Method
cpg	409.12	J/mol×K	831.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374270&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

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