3,4-Dichlorophenol, pentafluoropropionate

Other names: Pentafluoropropanoic acid, 3,4-dichlorophenyl ester
Inchi: InChI=1S/C9H3Cl2F5O2/c10-5-2-1-4(3-6(5)11)18-7(17)8(12,13)9(14,15)16/h1-3H
InchiKey: DVBDAOSDGGFSCU-UHFFFAOYSA-N
Formula: C9H3Cl2F5O2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 309.02
CAS: 959070-20-3

Physical Properties

Property code	Value	Unit	Source
gf	-1108.10	kJ/mol	Joback Method
hf	-1289.83	kJ/mol	Joback Method
hfus	24.08	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.096		Crippen Method
mcvol	154.680	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1081.00		NIST Webbook
tb	583.00	K	Joback Method
tc	783.87	K	Joback Method
tf	382.44	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.05	J/mol×K	583.00	Joback Method
cpg	361.02	J/mol×K	616.48	Joback Method
cpg	369.24	J/mol×K	649.96	Joback Method
cpg	376.76	J/mol×K	683.44	Joback Method
cpg	383.61	J/mol×K	716.91	Joback Method
cpg	389.85	J/mol×K	750.39	Joback Method
cpg	395.52	J/mol×K	783.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959070203&Units=SI

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