3-Chlorophenol, pentafluoropropionate

Inchi: InChI=1S/C9H4ClF5O2/c10-5-2-1-3-6(4-5)17-7(16)8(11,12)9(13,14)15/h1-4H
InchiKey: GENRORJFEYLBRE-UHFFFAOYSA-N
Formula: C9H4ClF5O2
SMILES: O=C(Oc1cccc(Cl)c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 274.57

Physical Properties

Property code	Value	Unit	Source
gf	-1086.54	kJ/mol	Joback Method
hf	-1262.62	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	45.43	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.443		Crippen Method
mcvol	142.440	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1038.00		NIST Webbook
tb	540.59	K	Joback Method
tc	736.00	K	Joback Method
tf	340.00	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.72	J/mol×K	540.59	Joback Method
cpg	339.95	J/mol×K	573.16	Joback Method
cpg	349.37	J/mol×K	605.73	Joback Method
cpg	358.04	J/mol×K	638.30	Joback Method
cpg	365.99	J/mol×K	670.87	Joback Method
cpg	373.27	J/mol×K	703.43	Joback Method
cpg	379.92	J/mol×K	736.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374283&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