4-Chloro-(2-hydroxyhexafluoroisopropyl)benzene

Inchi: InChI=1S/C9H5ClF6O/c10-6-3-1-5(2-4-6)7(17,8(11,12)13)9(14,15)16/h1-4,17H
InchiKey: BDVVJTPJVCAQGG-UHFFFAOYSA-N
Formula: C9H5ClF6O
SMILES: OC(c1ccc(Cl)cc1)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 278.58
CAS: 2010-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-1181.41	kJ/mol	Joback Method
hf	-1374.91	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.652		Crippen Method
mcvol	142.640	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	552.52	K	Joback Method
tc	732.39	K	Joback Method
tf	331.67	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.98	J/mol×K	552.52	Joback Method
cpg	361.56	J/mol×K	582.50	Joback Method
cpg	370.31	J/mol×K	612.48	Joback Method
cpg	378.30	J/mol×K	642.46	Joback Method
cpg	385.58	J/mol×K	672.43	Joback Method
cpg	392.23	J/mol×K	702.41	Joback Method
cpg	398.28	J/mol×K	732.39	Joback Method

Sources

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=C2010631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume