1,1,1,5,5,5-Hexafluoropentane-2,2,4,4-tetraol

Inchi: InChI=1S/C5H6F6O4/c6-4(7,8)2(12,13)1-3(14,15)5(9,10)11/h12-15H,1H2
InchiKey: BZMWYBPDQWRVHE-UHFFFAOYSA-N
Formula: C5H6F6O4
SMILES: OC(O)(CC(O)(O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 244.09
CAS: 66922-83-6

Physical Properties

Property code	Value	Unit	Source
gf	-1713.56	kJ/mol	Joback Method
hf	-1967.11	kJ/mol	Joback Method
hfus	13.88	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	-0.137		Crippen Method
mcvol	115.410	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	665.22	K	Joback Method
tc	819.88	K	Joback Method
tf	402.61	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.00	J/mol×K	665.22	Joback Method
cpg	362.79	J/mol×K	691.00	Joback Method
cpg	367.16	J/mol×K	716.77	Joback Method
cpg	371.17	J/mol×K	742.55	Joback Method
cpg	374.86	J/mol×K	768.33	Joback Method
cpg	378.26	J/mol×K	794.11	Joback Method
cpg	381.42	J/mol×K	819.88	Joback Method

Sources

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=C66922836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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