1,1,1,3,3,3-Hexafluoro-2-methoxy-2-propanol

Inchi: InChI=1S/C4H4F6O2/c1-12-2(11,3(5,6)7)4(8,9)10/h11H,1H3
InchiKey: FEKJGFZZVNCSRO-UHFFFAOYSA-N
Formula: C4H4F6O2
SMILES: COC(O)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 198.06
CAS: 662-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-1419.36	kJ/mol	Joback Method
hf	-1506.00	kJ/mol	NIST Webbook
hfl	-1579.00	kJ/mol	NIST Webbook
hfus	7.63	kJ/mol	Joback Method
hvap	72.80 ± 0.80	kJ/mol	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.446		Crippen Method
mcvol	89.580	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	391.45	K	Joback Method
tc	534.59	K	Joback Method
tf	228.69	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.47	J/mol×K	391.45	Joback Method
cpg	218.44	J/mol×K	415.31	Joback Method
cpg	225.91	J/mol×K	439.16	Joback Method
cpg	232.93	J/mol×K	463.02	Joback Method
cpg	239.49	J/mol×K	486.88	Joback Method
cpg	245.63	J/mol×K	510.73	Joback Method
cpg	251.36	J/mol×K	534.59	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=C662168&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
hfl:	Liquid phase 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