«alpha»-Hydroxyisobutyric acid, pentafluoropropionate

Inchi: InChI=1S/C7H7F5O4/c1-5(2,3(13)14)16-4(15)6(8,9)7(10,11)12/h1-2H3,(H,13,14)
InchiKey: IRMICLOUXGUURA-UHFFFAOYSA-N
Formula: C7H7F5O4
SMILES: CC(C)(OC(=O)C(F)(F)C(F)(F)F)C(=O)O
Mol. weight [g/mol]: 250.12

Physical Properties

Property code	Value	Unit	Source
gf	-1457.13	kJ/mol	Joback Method
hf	-1704.22	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.590		Crippen Method
mcvol	133.220	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	1005.00		NIST Webbook
tb	568.56	K	Joback Method
tc	736.53	K	Joback Method
tf	361.77	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.10	J/mol×K	568.56	Joback Method
cpg	363.58	J/mol×K	596.55	Joback Method
cpg	371.45	J/mol×K	624.55	Joback Method
cpg	378.76	J/mol×K	652.54	Joback Method
cpg	385.53	J/mol×K	680.54	Joback Method
cpg	391.80	J/mol×K	708.53	Joback Method
cpg	397.61	J/mol×K	736.53	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=U374315&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume