«alpha»-Hydroxyisobutyric acid, heptafluorobutyrate

Inchi: InChI=1S/C8H7F7O4/c1-5(2,3(16)17)19-4(18)6(9,10)7(11,12)8(13,14)15/h1-2H3,(H,16,1

InchiKey: OJGONUYELKIPPD-UHFFFAOYSA-N

Formula: C8H7F7O4

SMILES: CC(C)(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)O

Mol. weight [g/mol]: 300.13

Physical Properties

Property code	Value	Unit	Source
gf	-1835.49	kJ/mol	Joback Method
hf	-2125.83	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.226		Crippen Method
mcvol	150.850	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	1046.00		NIST Webbook
tb	586.75	K	Joback Method
tc	749.02	K	Joback Method
tf	376.64	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.90	J/mol×K	586.75	Joback Method
cpg	429.70	J/mol×K	613.80	Joback Method
cpg	437.83	J/mol×K	640.84	Joback Method
cpg	445.34	J/mol×K	667.89	Joback Method
cpg	452.26	J/mol×K	694.93	Joback Method
cpg	458.65	J/mol×K	721.98	Joback Method
cpg	464.53	J/mol×K	749.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374314&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

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