(+-)-3-hydroxybutyric acid, heptafluorobutyrate

Inchi: InChI=1S/C8H7F7O4/c1-3(2-4(16)17)19-5(18)6(9,10)7(11,12)8(13,14)15/h3H,2H2,1H3,(

InchiKey: BTCLXOUNCZJBIF-UHFFFAOYSA-N

Formula: C8H7F7O4

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

Mol. weight [g/mol]: 300.13

Physical Properties

Property code	Value	Unit	Source
gf	-1840.77	kJ/mol	Joback Method
hf	-2122.36	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.226		Crippen Method
mcvol	150.850	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
tb	589.54	K	Joback Method
tc	747.72	K	Joback Method
tf	359.22	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.70	J/mol×K	589.54	Joback Method
cpg	426.33	J/mol×K	615.90	Joback Method
cpg	434.38	J/mol×K	642.27	Joback Method
cpg	441.88	J/mol×K	668.63	Joback Method
cpg	448.86	J/mol×K	694.99	Joback Method
cpg	455.35	J/mol×K	721.36	Joback Method
cpg	461.38	J/mol×K	747.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374309&Units=SI

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