(+-)-3-hydroxybutyric acid, trifluoroacetate

Inchi: InChI=1S/C6H7F3O4/c1-3(2-4(10)11)13-5(12)6(7,8)9/h3H,2H2,1H3,(H,10,11)
InchiKey: VOYYDTLQLYVTGM-UHFFFAOYSA-N
Formula: C6H7F3O4
SMILES: CC(CC(=O)O)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 200.11

Physical Properties

Property code	Value	Unit	Source
gf	-1084.05	kJ/mol	Joback Method
hf	-1279.14	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	57.40	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.955		Crippen Method
mcvol	115.590	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1001.00		NIST Webbook
rinpol	1001.00		NIST Webbook
tb	553.16	K	Joback Method
tc	722.48	K	Joback Method
tf	329.48	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.13	J/mol×K	553.16	Joback Method
cpg	294.87	J/mol×K	581.38	Joback Method
cpg	302.20	J/mol×K	609.60	Joback Method
cpg	309.13	J/mol×K	637.82	Joback Method
cpg	315.66	J/mol×K	666.04	Joback Method
cpg	321.81	J/mol×K	694.26	Joback Method
cpg	327.60	J/mol×K	722.48	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=U374311&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