(+-)-3-hydroxybutyric acid, pentafluoropropionate

Inchi: InChI=1S/C7H7F5O4/c1-3(2-4(13)14)16-5(15)6(8,9)7(10,11)12/h3H,2H2,1H3,(H,13,14)
InchiKey: ZTPLUBBHELQQIZ-UHFFFAOYSA-N
Formula: C7H7F5O4
SMILES: CC(CC(=O)O)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 250.12

Physical Properties

Property code	Value	Unit	Source
gf	-1462.41	kJ/mol	Joback Method
hf	-1700.75	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	56.69	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.590		Crippen Method
mcvol	133.220	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	1020.00		NIST Webbook
tb	571.35	K	Joback Method
tc	734.50	K	Joback Method
tf	344.35	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.78	J/mol×K	571.35	Joback Method
cpg	360.05	J/mol×K	598.54	Joback Method
cpg	367.80	J/mol×K	625.73	Joback Method
cpg	375.07	J/mol×K	652.92	Joback Method
cpg	381.88	J/mol×K	680.11	Joback Method
cpg	388.24	J/mol×K	707.31	Joback Method
cpg	394.18	J/mol×K	734.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374310&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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