(+-)-2-Hydroxyoctanoic acid, trifluoroacetate

Inchi: InChI=1S/C10H15F3O4/c1-2-3-4-5-6-7(8(14)15)17-9(16)10(11,12)13/h7H,2-6H2,1H3,(H,
InchiKey: GBAXXYUPUIVJAF-UHFFFAOYSA-N
Formula: C10H15F3O4
SMILES: CCCCCCC(OC(=O)C(F)(F)F)C(=O)O
Mol. weight [g/mol]: 256.22

Physical Properties

Property code	Value	Unit	Source
gf	-1050.37	kJ/mol	Joback Method
hf	-1361.70	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	66.30	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.516		Crippen Method
mcvol	171.950	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1352.00		NIST Webbook
tb	644.68	K	Joback Method
tc	811.81	K	Joback Method
tf	374.56	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.41	J/mol×K	644.68	Joback Method
cpg	485.09	J/mol×K	672.54	Joback Method
cpg	495.22	J/mol×K	700.39	Joback Method
cpg	504.81	J/mol×K	728.25	Joback Method
cpg	513.88	J/mol×K	756.10	Joback Method
cpg	522.45	J/mol×K	783.96	Joback Method
cpg	530.53	J/mol×K	811.81	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=U374242&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