(+-)-2-Hydroxyoctanoic acid, pentafluoropropionate

Inchi: InChI=1S/C11H15F5O4/c1-2-3-4-5-6-7(8(17)18)20-9(19)10(12,13)11(14,15)16/h7H,2-6H

InchiKey: AXGMGBCYGANCAG-UHFFFAOYSA-N

Formula: C11H15F5O4

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

Mol. weight [g/mol]: 306.23

Physical Properties

Property code	Value	Unit	Source
gf	-1428.73	kJ/mol	Joback Method
hf	-1783.31	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	65.60	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.151		Crippen Method
mcvol	189.580	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	1369.00		NIST Webbook
tb	662.87	K	Joback Method
tc	826.53	K	Joback Method
tf	389.43	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.12	J/mol×K	662.87	Joback Method
cpg	554.90	J/mol×K	690.15	Joback Method
cpg	565.06	J/mol×K	717.42	Joback Method
cpg	574.64	J/mol×K	744.70	Joback Method
cpg	583.65	J/mol×K	771.97	Joback Method
cpg	592.13	J/mol×K	799.25	Joback Method
cpg	600.11	J/mol×K	826.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374329&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