2-Hydroxyisocaproic acid, pentafluoropropionate

Inchi: InChI=1S/C9H11F5O4/c1-4(2)3-5(6(15)16)18-7(17)8(10,11)9(12,13)14/h4-5H,3H2,1-2H3

InchiKey: XEXKYFPORBOREK-UHFFFAOYSA-N

Formula: C9H11F5O4

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

Mol. weight [g/mol]: 278.17

Physical Properties

Property code	Value	Unit	Source
gf	-1448.01	kJ/mol	Joback Method
hf	-1747.31	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.226		Crippen Method
mcvol	161.400	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
tb	616.67	K	Joback Method
tc	781.60	K	Joback Method
tf	351.89	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.46	J/mol×K	616.67	Joback Method
cpg	455.24	J/mol×K	644.16	Joback Method
cpg	464.43	J/mol×K	671.65	Joback Method
cpg	473.07	J/mol×K	699.14	Joback Method
cpg	481.17	J/mol×K	726.62	Joback Method
cpg	488.76	J/mol×K	754.11	Joback Method
cpg	495.87	J/mol×K	781.60	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=U374427&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