2-Hydroxyisocaproic acid, trifluoroacetate

Inchi: InChI=1S/C8H11F3O4/c1-4(2)3-5(6(12)13)15-7(14)8(9,10)11/h4-5H,3H2,1-2H3,(H,12,13
InchiKey: DZXQBBALFIMLBZ-UHFFFAOYSA-N
Formula: C8H11F3O4
SMILES: CC(C)CC(OC(=O)C(F)(F)F)C(=O)O
Mol. weight [g/mol]: 228.17

Physical Properties

Property code	Value	Unit	Source
gf	-1069.65	kJ/mol	Joback Method
hf	-1325.70	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	61.46	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.591		Crippen Method
mcvol	143.770	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
tb	598.48	K	Joback Method
tc	768.75	K	Joback Method
tf	337.02	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.00	J/mol×K	598.48	Joback Method
cpg	387.53	J/mol×K	626.86	Joback Method
cpg	396.55	J/mol×K	655.24	Joback Method
cpg	405.07	J/mol×K	683.62	Joback Method
cpg	413.12	J/mol×K	712.00	Joback Method
cpg	420.70	J/mol×K	740.37	Joback Method
cpg	427.83	J/mol×K	768.75	Joback Method

Sources

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=U374426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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