5,5,5-Trifluoroleucine

Inchi: InChI=1S/C6H10F3NO2/c1-3(6(7,8)9)2-4(10)5(11)12/h3-4H,2,10H2,1H3,(H,11,12)
InchiKey: XFGVJLGVINCWDP-UHFFFAOYSA-N
Formula: C6H10F3NO2
SMILES: CC(CC(N)C(=O)O)C(F)(F)F
Mol. weight [g/mol]: 185.14

Physical Properties

Property code	Value	Unit	Source
gf	-786.12	kJ/mol	Joback Method
hf	-1005.83	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.987		Crippen Method
mcvol	118.130	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1042.00		NIST Webbook
tb	548.96	K	Joback Method
tc	723.21	K	Joback Method
tf	325.58	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.35	J/mol×K	548.96	Joback Method
cpg	313.28	J/mol×K	578.00	Joback Method
cpg	321.69	J/mol×K	607.04	Joback Method
cpg	329.60	J/mol×K	636.08	Joback Method
cpg	337.04	J/mol×K	665.13	Joback Method
cpg	344.03	J/mol×K	694.17	Joback Method
cpg	350.59	J/mol×K	723.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221926&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