Norleucine, N-trifluoroacetyl, 1-methylethyl ester

Inchi: InChI=1S/C11H18F3NO3/c1-4-5-6-8(9(16)18-7(2)3)15-10(17)11(12,13)14/h7-8H,4-6H2,1

InchiKey: HYRZCTVPACSGPE-UHFFFAOYSA-N

Formula: C11H18F3NO3

SMILES: CCCCC(NC(=O)C(F)(F)F)C(=O)OC(C)C

Mol. weight [g/mol]: 269.26

Physical Properties

Property code	Value	Unit	Source
gf	-818.18	kJ/mol	Joback Method
hf	-1181.92	kJ/mol	Joback Method
hfus	28.51	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.175		Crippen Method
mcvol	190.150	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	1203.00		NIST Webbook
rinpol	1203.00		NIST Webbook
tb	625.11	K	Joback Method
tc	800.08	K	Joback Method
tf	362.67	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.28	J/mol×K	625.11	Joback Method
cpg	533.65	J/mol×K	654.27	Joback Method
cpg	546.31	J/mol×K	683.43	Joback Method
cpg	558.29	J/mol×K	712.59	Joback Method
cpg	569.59	J/mol×K	741.76	Joback Method
cpg	580.25	J/mol×K	770.92	Joback Method
cpg	590.29	J/mol×K	800.08	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=R84445&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