leucine, trifluoroacetyl-isopropyl ester

Other names: Leucine, N-trifluoroacetyl, 1-methylethyl ester
Inchi: InChI=1S/C11H18F3NO3/c1-6(2)5-8(9(16)18-7(3)4)15-10(17)11(12,13)14/h6-8H,5H2,1-4
InchiKey: MGXDWBLMYIJEEM-UHFFFAOYSA-N
Formula: C11H18F3NO3
SMILES: CC(C)CC(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	-820.62	kJ/mol	Joback Method
hf	-1187.20	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	57.51	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.031		Crippen Method
mcvol	190.150	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1148.00		NIST Webbook
rinpol	1236.00		NIST Webbook
tb	624.67	K	Joback Method
tc	802.39	K	Joback Method
tf	347.67	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.72	J/mol×K	624.67	Joback Method
cpg	534.34	J/mol×K	654.29	Joback Method
cpg	547.23	J/mol×K	683.91	Joback Method
cpg	559.39	J/mol×K	713.53	Joback Method
cpg	570.86	J/mol×K	743.15	Joback Method
cpg	581.66	J/mol×K	772.77	Joback Method
cpg	591.81	J/mol×K	802.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R84431&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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