Norvaline, N-trifluoroacetyl, 1-methylethyl ester

Other names: norvaline, trifluoroacetyl-isopropyl ester
Inchi: InChI=1S/C10H16F3NO3/c1-4-5-7(8(15)17-6(2)3)14-9(16)10(11,12)13/h6-7H,4-5H2,1-3H
InchiKey: DRNUDDOESVDZJT-UHFFFAOYSA-N
Formula: C10H16F3NO3
SMILES: CCCC(NC(=O)C(F)(F)F)C(=O)OC(C)C
Mol. weight [g/mol]: 255.23

Physical Properties

Property code	Value	Unit	Source
gf	-826.60	kJ/mol	Joback Method
hf	-1161.28	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.785		Crippen Method
mcvol	176.060	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	602.23	K	Joback Method
tc	778.24	K	Joback Method
tf	351.40	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.11	J/mol×K	602.23	Joback Method
cpg	482.91	J/mol×K	631.57	Joback Method
cpg	495.04	J/mol×K	660.90	Joback Method
cpg	506.51	J/mol×K	690.24	Joback Method
cpg	517.34	J/mol×K	719.57	Joback Method

cpg	527.54	J/mol×K	748.91	Joback Method
cpg	537.15	J/mol×K	778.24	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=R84459&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