4,4,4-Trifluorovaline

Inchi: InChI=1S/C5H8F3NO2/c1-2(5(6,7)8)3(9)4(10)11/h2-3H,9H2,1H3,(H,10,11)
InchiKey: BAOLXXJPOPIBKA-UHFFFAOYSA-N
Formula: C5H8F3NO2
SMILES: CC(C(N)C(=O)O)C(F)(F)F
Mol. weight [g/mol]: 171.12
CAS: 16063-79-9

Physical Properties

Property code	Value	Unit	Source
gf	-794.54	kJ/mol	Joback Method
hf	-985.19	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Joback Method
hvap	56.27	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.597		Crippen Method
mcvol	104.040	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	979.00		NIST Webbook
rinpol	979.00		NIST Webbook
tb	526.08	K	Joback Method
tc	701.79	K	Joback Method
tf	314.31	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.19	J/mol×K	526.08	Joback Method
cpg	269.25	J/mol×K	555.37	Joback Method
cpg	276.83	J/mol×K	584.65	Joback Method
cpg	283.94	J/mol×K	613.94	Joback Method
cpg	290.61	J/mol×K	643.22	Joback Method
cpg	296.86	J/mol×K	672.51	Joback Method
cpg	302.71	J/mol×K	701.79	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=C16063799&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