3-fluronorvaline, threo

Inchi: InChI=1S/C5H10FNO2/c1-2-3(6)4(7)5(8)9/h3-4H,2,7H2,1H3,(H,8,9)/t3-,4+/m0/s1
InchiKey: FFBPWYMQRDXRER-IUYQGCFVSA-N
Formula: C5H10FNO2
SMILES: CCC(F)C(N)C(=O)O
Mol. weight [g/mol]: 135.14

Physical Properties

Property code	Value	Unit	Source
gf	-407.76	kJ/mol	Joback Method
hf	-584.22	kJ/mol	Joback Method
hfus	15.62	kJ/mol	Joback Method
hvap	59.20	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.146		Crippen Method
mcvol	100.500	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
tb	530.77	K	Joback Method
tc	713.08	K	Joback Method
tf	310.71	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.72	J/mol×K	530.77	Joback Method
cpg	248.99	J/mol×K	561.15	Joback Method
cpg	256.85	J/mol×K	591.54	Joback Method
cpg	264.33	J/mol×K	621.92	Joback Method
cpg	271.42	J/mol×K	652.31	Joback Method
cpg	278.15	J/mol×K	682.69	Joback Method
cpg	284.52	J/mol×K	713.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221911&Units=SI

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

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