3-Fluorovaline

Inchi: InChI=1S/C5H10FNO2/c1-5(2,6)3(7)4(8)9/h3H,7H2,1-2H3,(H,8,9)
InchiKey: ZFUKCHCGMBNYHH-UHFFFAOYSA-N
Formula: C5H10FNO2
SMILES: CC(C)(F)C(N)C(=O)O
Mol. weight [g/mol]: 135.14

Physical Properties

Property code	Value	Unit	Source
gf	-402.48	kJ/mol	Joback Method
hf	-587.69	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.146		Crippen Method
mcvol	100.500	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	1021.00		NIST Webbook
tb	527.98	K	Joback Method
tc	717.05	K	Joback Method
tf	328.13	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.12	J/mol×K	527.98	Joback Method
cpg	252.75	J/mol×K	559.49	Joback Method
cpg	260.86	J/mol×K	591.00	Joback Method
cpg	268.46	J/mol×K	622.52	Joback Method
cpg	275.59	J/mol×K	654.03	Joback Method
cpg	282.27	J/mol×K	685.54	Joback Method
cpg	288.53	J/mol×K	717.05	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=R221897&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