3-Fluoroalanine

Inchi: InChI=1S/C3H6FNO2/c4-1-2(5)3(6)7/h2H,1,5H2,(H,6,7)
InchiKey: UYTSRQMXRROFPU-UHFFFAOYSA-N
Formula: C3H6FNO2
SMILES: NC(CF)C(=O)O
Mol. weight [g/mol]: 107.08

Physical Properties

Property code	Value	Unit	Source
gf	-422.16	kJ/mol	Joback Method
hf	-537.66	kJ/mol	Joback Method
hfus	13.97	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	0.42		Crippen Method
logp	-0.632		Crippen Method
mcvol	72.320	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
rinpol	922.00		NIST Webbook
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tb	485.45	K	Joback Method
tc	667.76	K	Joback Method
tf	303.17	K	Joback Method
vc	0.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.74	J/mol×K	485.45	Joback Method
cpg	165.55	J/mol×K	515.83	Joback Method
cpg	171.08	J/mol×K	546.22	Joback Method
cpg	176.34	J/mol×K	576.60	Joback Method
cpg	181.34	J/mol×K	606.99	Joback Method
cpg	186.08	J/mol×K	637.37	Joback Method
cpg	190.57	J/mol×K	667.76	Joback Method

Sources

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=R221862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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