

2-Amino-3-fluorobutyric acid, threo

Inchi:	InChI=1S/C4H8FNO2/c1-2(5)3(6)4(7)8/h2-3H,6H2,1H3,(H,7,8)/t2-,3+/m0/s1
InchiKey:	HJVQOHDATXHIJL-STHAYSLISA-N
Formula:	C4H8FNO2
SMILES:	CC(F)C(N)C(=O)O
Mol. weight [g/mol]:	121.11

Physical Properties

Property code	Value	Unit	Source
gf	-416.18	kJ/mol	Joback Method
hf	-563.58	kJ/mol	Joback Method
hfus	13.03	kJ/mol	Joback Method
hvap	56.97	kJ/mol	Joback Method
log10ws	-0.11		Crippen Method
logp	-0.244		Crippen Method
mcvol	86.410	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
tb	507.89	K	Joback Method
tc	692.13	K	Joback Method
tf	299.44	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.36	J/molxK	507.89	Joback Method
cpg	206.55	J/molxK	538.60	Joback Method
cpg	213.40	J/molxK	569.30	Joback Method
cpg	219.90	J/molxK	600.01	Joback Method
cpg	226.07	J/molxK	630.72	Joback Method
cpg	231.91	J/molxK	661.43	Joback Method
cpg	237.44	J/molxK	692.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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