

# 3-Fluoronorleucine, threo

<b>Inchi:</b>	InChI=1S/C6H12FNO2/c1-3(2)4(7)5(8)6(9)10/h3-5H,8H2,1-2H3,(H,9,10)/t4-,5+/m0/s1
<b>InchiKey:</b>	SYEUPUMYWNMWKJ-CRCLSJGQSA-N
<b>Formula:</b>	C6H12FNO2
<b>SMILES:</b>	CC(C)C(F)C(N)C(=O)O
<b>Mol. weight [g/mol]:</b>	149.16

## Physical Properties

Property code	Value	Unit	Source
gf	-401.78	kJ/mol	Joback Method
hf	-610.14	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.392		Crippen Method
mcvol	114.590	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
rinpol	1152.00		NIST Webbook
tb	553.21	K	Joback Method
tc	737.17	K	Joback Method
tf	306.98	K	Joback Method
vc	0.425	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.41	J/molxK	553.21	Joback Method
cpg	293.87	J/molxK	583.87	Joback Method
cpg	302.87	J/molxK	614.53	Joback Method
cpg	311.40	J/molxK	645.19	Joback Method
cpg	319.49	J/molxK	675.85	Joback Method
cpg	327.16	J/molxK	706.51	Joback Method
cpg	334.40	J/molxK	737.17	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R221882&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R221882&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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