

Pregabalin

Other names:	(5)-3(aminomethyl)-5-Methyl Hexanoic Acid (Pregabaline Crude) (S)-3-(Aminomethyl)-5-methylhexanoic acid 3-(Amino methyl)-5-methyl hexanoic acid (racemic) Hexanoic acid, 3-(aminomethyl)-5-methyl-, (3S)- Lyrica
Inchi:	InChI=1S/C8H17NO2/c1-6(2)3-7(5-9)4-8(10)11/h6-7H,3-5,9H2,1-2H3,(H,10,11)
InchiKey:	AYXYPKUFHZROOJ-UHFFFAOYSA-N
Formula:	C8H17NO2
SMILES:	CC(C)CC(CN)CC(=O)O
Mol. weight [g/mol]:	159.23
CAS:	148553-50-8

Physical Properties

Property code	Value	Unit	Source
gf	-187.69	kJ/mol	Joback Method
hf	-450.03	kJ/mol	Joback Method
hfus	20.31	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.082		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	600.14	K	Joback Method
tc	784.87	K	Joback Method
tf	343.93	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.79	J/molxK	600.14	Joback Method
cpg	379.16	J/molxK	630.93	Joback Method
cpg	389.97	J/molxK	661.72	Joback Method
cpg	400.23	J/molxK	692.50	Joback Method

cpg	409.98	J/mol×K	723.29	Joback Method
cpg	419.21	J/mol×K	754.08	Joback Method
cpg	427.96	J/mol×K	784.87	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of (S)-3-(Aminomethyl)-5-Methylhexanoic Acid in Pure and Binary Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.5b00736
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148553508&Units=SI
	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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