

2-(1-(aminomethyl)cyclohexyl)acetic acid

Other names:	gabapentin
Inchi:	InChI=1S/C9H17NO2/c10-7-9(6-8(11)12)4-2-1-3-5-9/h1-7,10H2,(H,11,12)
InchiKey:	UGJMXCAKCUNAIE-UHFFFAOYSA-N
Formula:	C9H17NO2
SMILES:	<chem>NCC1(CC(=O)O)CCCCC1</chem>
Mol. weight [g/mol]:	171.24

Physical Properties

Property code	Value	Unit	Source
gf	-155.43	kJ/mol	Joback Method
hf	-390.55	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	68.97	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.370		Crippen Method
mvol	144.230	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	643.69	K	Joback Method
tc	855.70	K	Joback Method
tf	416.48	K	Joback Method
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.93	J/mol×K	643.69	Joback Method
cpg	415.54	J/mol×K	679.02	Joback Method
cpg	428.43	J/mol×K	714.36	Joback Method
cpg	440.70	J/mol×K	749.69	Joback Method
cpg	452.48	J/mol×K	785.03	Joback Method
cpg	463.86	J/mol×K	820.36	Joback Method
cpg	474.97	J/mol×K	855.70	Joback Method

rhos	1239.00	kg/m ³	293.00	Thermodynamic and molecular investigation into the solubility, stability and self-assembly of gabapentin anhydrate and hydrate
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic and molecular investigation into the solubility, stability and self-assembly of gabapentin anhydrate and hydrate:	https://www.doi.org/10.1016/j.jct.2017.05.041
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	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
rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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