

N-Acetyl-L-glutamic acid

Other names:	2-acetamidopentanedioic acid Acetyl-L-glutamic acid L-Glutamic acid, N-acetyl- N-acetylglutamic acid
Inchi:	InChI=1S/C7H11NO5/c1-4(9)8-5(7(12)13)2-3-6(10)11/h5H,2-3H2,1H3,(H,8,9)(H,10,11)(H,12,13)
InchiKey:	RFMMMVDNIPUKGG-RXMQYKEDSA-N
Formula:	C7H11NO5
SMILES:	CC(=O)NC(CCC(=O)O)C(=O)O
Mol. weight [g/mol]:	189.17
CAS:	1188-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-565.39	kJ/mol	Joback Method
hf	-781.82	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	90.82	kJ/mol	Joback Method
log10ws	-0.71		Aqueous Solubility Prediction Method
logp	-0.559		Crippen Method
mcvol	135.920	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	755.26	K	Joback Method
tc	941.96	K	Joback Method
tf	477.74	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.61	J/molxK	755.26	Joback Method
cpg	384.78	J/molxK	786.38	Joback Method
cpg	391.49	J/molxK	817.49	Joback Method
cpg	397.75	J/molxK	848.61	Joback Method

cpg	403.58	J/mol×K	879.72	Joback Method
cpg	408.99	J/mol×K	910.84	Joback Method
cpg	414.00	J/mol×K	941.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1188370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
hvp:	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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