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
InchiKey: RFMMMVDNIPUKGG-UHFFFAOYSA-N
Formula: C7H11NO5
SMILES: CC(=O)N[C@@H](CCC(=O)O)C(=O)O
Mol. weight [g/mol]: 189.17

Physical Properties

Property code	Value	Unit	Source
hfus	28.44	kJ/mol	Joback Method
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-0.71		Aqueous Solubility Prediction Method
logp	-0.559		Crippen Method
mcvol	135.920	ml/mol	McGowan Method
tf	437.93	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1188370&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point