

4-Acetamidobutyric acid

Other names:	N-Acetyl-«gamma»-aminobutyric acid N-Acetyl-«gamma»-amino-n-butyric acid Butanoic acid, 4-(acetlamino)-«gamma»-Acetylaminobutyric acid Butyric acid, 4-acetamido-DF 469 N-Acetyl-4-aminobutanoic acid N-Acetyl-4-aminobutyric acid NSC 27423
Inchi:	InChI=1S/C6H11NO3/c1-5(8)7-4-2-3-6(9)10/h2-4H2,1H3,(H,7,8)(H,9,10)
InchiKey:	UZTFMUBKZQVKLK-UHFFFAOYSA-N
Formula:	C6H11NO3
SMILES:	CC(=O)NCCCC(=O)O
Mol. weight [g/mol]:	145.16
CAS:	3025-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-305.63	kJ/mol	Joback Method
hf	-491.09	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	65.56	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	-0.013		Crippen Method
mcvol	114.390	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	586.77	K	Joback Method
tc	769.09	K	Joback Method
tf	370.72	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	278.84	J/mol×K	586.77	Joback Method
cpg	287.39	J/mol×K	617.16	Joback Method
cpg	295.52	J/mol×K	647.54	Joback Method
cpg	303.24	J/mol×K	677.93	Joback Method
cpg	310.56	J/mol×K	708.32	Joback Method
cpg	317.49	J/mol×K	738.71	Joback Method
cpg	324.04	J/mol×K	769.09	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3025965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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