4-(ACETYLAMINO)BUTYRIC ACID

Other names:	N-Acetyl-«gamma»-aminobutyric acid
	N-Acetyl-«gamma»-amino-n-butyric acid
	Butanoic acid, 4-(acetylamino)-
	«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

Physical Properties

Property code	Value	Unit	Source
gf	-305.63	kJ/mol	Joback Method
hf	-656.72	kJ/mol	Cheméo Relay (1.0)
hfus	23.68	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	0.15		Cheméo Relay (1.0)
logp	-0.013		Crippen Method
mcvol	114.390	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	533.50	K	Cheméo Relay (1.0)
tc	750.73	K	Cheméo Relay (1.0)
tf	384.30	K	Cheméo Relay (1.0)
vc	0.417	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3025965&Units=SI
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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
ie:	Ionization energy
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