N-ACETYLNORVALINE METHYLAMIDE

Other names: 2-(acetylamino)-N-methylpentanamide
N-Acetylnorvaline-N'-methylamide (DL)
N-acetyl-N'-methyl-DL-norvalinamide
Inchi: InChI=1S/C8H16N2O2/c1-4-5-7(8(12)9-3)10-6(2)11/h7H,4-5H2,1-3H3,(H,9,12)(H,10,11)
InchiKey: SKSIAIMVWBILBT-UHFFFAOYSA-N
Formula: C8H16N2O2
SMILES: CCCC(NC(C)=O)C(=O)NC
Mol. weight [g/mol]: 172.23

Physical Properties

Property code	Value	Unit	Source
hfus	26.35	kJ/mol	Joback Method
log10ws	-0.88		Cheméo Relay (1.0)
logp	0.037		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
tf	361.12	K	Cheméo Relay (1.0)
tt	432.29	K	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.91	J/mol×K	590.08	Joback Method
cpg	382.32	J/mol×K	622.20	Joback Method
cpg	394.08	J/mol×K	654.32	Joback Method
cpg	405.21	J/mol×K	686.44	Joback Method
cpg	415.74	J/mol×K	718.56	Joback Method
cpg	425.66	J/mol×K	750.68	Joback Method
cpg	435.02	J/mol×K	782.80	Joback Method
cps	239.69	J/mol×K	298.00	NIST Webbook

Sources

Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups:	https://www.doi.org/10.1016/j.jct.2013.12.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33067468&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
cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature