1-acetyl-N-methylprolinamide

Other names:	1-acetyl-N-methylpyrrolidine-2-carboxamide
	acetylproline-N-methylamide
Inchi:	InChI=1S/C8H14N2O2/c1-6(11)10-5-3-4-7(10)8(12)9-2/h7H,3-5H2,1-2H3,(H,9,12)
InchiKey:	DPDXFAYSYVRXMF-UHFFFAOYSA-N
Formula:	C8H14N2O2
SMILES:	CNC(=O)C1CCCN1C(C)=O
Mol. weight [g/mol]:	170.21

Physical Properties

Property code	Value	Unit	Source
hfus	26.06	kJ/mol	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
log10ws	-0.49		Crippen Method
logp	-0.257		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
tt	378.12	K	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
tt:	Triple Point Temperature