N-acetyl-N'-methyl-L-alpha-tyrosinamide

Inchi: InChI=1S/C12H16N2O3/c1-8(15)14-11(12(17)13-2)7-9-3-5-10(16)6-4-9/h3-6,11,16H,7H2
InchiKey: KHRMBHFDICMQHO-UHFFFAOYSA-N
Formula: C12H16N2O3
SMILES: CNC(=O)C(Cc1ccc(O)cc1)NC(C)=O
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	-73.55	kJ/mol	Joback Method
hf	-355.29	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	83.57	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.185		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	788.90	K	Joback Method
tc	1014.84	K	Joback Method
tf	199.00	K	Studies of heterogeneous interactions between N-acetyl-N'-methyl-L-a-amino acid amides and urea molecules in water at 298.15 K
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.60	J/mol×K	788.90	Joback Method
cpg	548.36	J/mol×K	826.56	Joback Method
cpg	559.40	J/mol×K	864.21	Joback Method
cpg	569.81	J/mol×K	901.87	Joback Method
cpg	579.69	J/mol×K	939.53	Joback Method
cpg	589.13	J/mol×K	977.18	Joback Method
cpg	598.22	J/mol×K	1014.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Studies of heterogeneous interactions between N-acetyl-N'-methyl-L-a-amino acid amides and urea molecules in water at 298.15 K:	https://www.doi.org/10.1016/j.tca.2009.12.017
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
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