N-(2-PYRIDYL)ACETAMIDE

Inchi: InChI=1S/C7H8N2O/c1-6(10)9-7-4-2-3-5-8-7/h2-5H,1H3,(H,8,9,10)
InchiKey: QROKOTBWFZITJZ-UHFFFAOYSA-N
Formula: C7H8N2O
SMILES: CC(=O)Nc1ccccn1
Mol. weight [g/mol]: 136.15

Physical Properties

Property code	Value	Unit	Source
hvap	71.76	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-0.74		Cheméo Relay (1.0)
logp	1.040		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
tb	530.66	K	Cheméo Relay (1.0)
tf	351.04	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C5231969
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point