NICOTINAMIDE

Inchi: InChI=1S/C6H6N2O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)
InchiKey: DFPAKSUCGFBDDF-UHFFFAOYSA-N
Formula: C6H6N2O
SMILES: NC(=O)c1cccnc1
Mol. weight [g/mol]: 122.13

Physical Properties

Property code	Value	Unit	Source
hf	-81.84	kJ/mol	Cheméo Relay (1.0)
hvap	66.13	kJ/mol	Cheméo Relay (1.0)
ie	9.64	eV	Cheméo Relay (1.0)
log10ws	0.61		Aqueous Solubility Prediction Method
log10ws	0.61		Estimated Solubility Method
logp	0.181		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
tb	534.63	K	Cheméo Relay (1.0)
tf	403.05	K	Aqueous Solubility Prediction Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C98920
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point