N,N-dimethylnicotinamide

Other names: N,N-dimethyl-3-pyridinecarboxamide
Inchi: InChI=1S/C8H10N2O/c1-10(2)8(11)7-4-3-5-9-6-7/h3-6H,1-2H3
InchiKey: FJEVKYZLIRAAKE-UHFFFAOYSA-N
Formula: C8H10N2O
SMILES: CN(C)C(=O)c1cccnc1
Mol. weight [g/mol]: 150.18

Physical Properties

Property code	Value	Unit	Source
af	0.4748		Cheméo Relay (1.0)
gf	151.24	kJ/mol	Cheméo Relay (1.0, beta)
hf	-30.41	kJ/mol	Cheméo Relay (1.0)
hvap	66.19	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-0.11		Cheméo Relay (1.0)
logp	0.783		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3370.72	kPa	Cheméo Relay (1.0, beta)
tb	543.96	K	Cheméo Relay (1.0)
tc	761.08	K	Cheméo Relay (1.0)
tf	317.30	K	Thermodynamic study of nicotinamide, N-methylnicotinamide and N,N-dimethylnicotinamide: Vapour pressures, phase diagrams, and hydrogen bonds
vc	0.457	m3/kmol	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):
Thermodynamic study of nicotinamide, N-methylnicotinamide and N,N-dimethylnicotinamide: Vapour pressures, phase diagrams, and hydrogen bonds: https://www.doi.org/10.1016/j.jct.2014.11.001

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume