

N-methylnicotinamide

Other names:	3-(N-methylcarbamoyl)pyridine N-methyl-3-pyridinecarboxamide
Inchi:	InChI=1S/C7H8N2O/c1-8-7(10)6-3-2-4-9-5-6/h2-5H,1H3,(H,8,10)
InchiKey:	ZYVXHFWBYUDDBM-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	CNC(=O)c1cccnc1
Mol. weight [g/mol]:	136.15

Physical Properties

Property code	Value	Unit	Source
af	0.4943		Cheméo Relay (1.0)
gf	101.14	kJ/mol	Cheméo Relay (1.0, beta)
hf	-51.17	kJ/mol	Cheméo Relay (1.0)
hvap	70.03	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-0.28		Cheméo Relay (1.0)
logp	0.441		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4391.17	kPa	Cheméo Relay (1.0, beta)
tb	533.40	K	Cheméo Relay (1.0)
tc	796.54	K	Cheméo Relay (1.0)
tf	379.10	K	Thermodynamic study of nicotinamide, N-methylnicotinamide and N,N-dimethylnicotinamide: Vapour pressures, phase diagrams, and hydrogen bonds
vc	0.388	m ³ /kmol	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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, <https://www.doi.org/10.1016/j.jct.2014.11.001>

N-methylnicotinamide and
N,N-dimethylnicotinamide: Vapour
pressures, phase diagrams, and
hydrogen bonds:

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

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