

N-Methyl-4-nitrophthalimide

Inchi:	InChI=1S/C9H6N2O4/c1-10-8(12)6-3-2-5(11(14)15)4-7(6)9(10)13/h2-4H,1H3
InchiKey:	JBCHWGTZAAZJKG-UHFFFAOYSA-N
Formula:	C9H6N2O4
SMILES:	CN1C(=O)c2ccc([N+](=O)[O-])cc2C1=O
Mol. weight [g/mol]:	206.16
CAS:	41663-84-7

Physical Properties

Property code	Value	Unit	Source
hf	-233.79	kJ/mol	Cheméo Relay (1.0)
hvap	82.49	kJ/mol	Cheméo Relay (1.0)
ie	10.21	eV	Cheméo Relay (1.0)
log10ws	-2.74		Cheméo Relay (1.0)
logp	0.821		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
tb	587.28	K	Cheméo Relay (1.0)
tf	369.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
t_b:	Normal Boiling Point Temperature
t_f:	Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/107-258-7/N-Methyl-4-nitrophthalimide.pdf>

Generated by Cheméo on 2026-10-28 16:17:43.502697456 +0000 UTC m=+69306.565598891.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.