

N-hydroxyphthalimide

Other names:	phthalimide, N-hydroxy-
Inchi:	InChI=1S/C8H5NO3/c10-7-5-3-1-2-4-6(5)8(11)9(7)12/h1-4,12H
InchiKey:	CFMZSMGAMPBRBE-UHFFFAOYSA-N
Formula:	C8H5NO3
SMILES:	O=C1c2ccccc2C(=O)N1O
Mol. weight [g/mol]:	163.13

Physical Properties

Property code	Value	Unit	Source
hf	-269.74	kJ/mol	Cheméo Relay (1.0)
ie	9.71	eV	Cheméo Relay (1.0)
log10ws	-1.53		Cheméo Relay (1.0)
logp	0.672		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4845.25	kPa	Cheméo Relay (1.0, beta)
tb	579.57	K	Cheméo Relay (1.0)
tc	895.19	K	Cheméo Relay (1.0)
tf	444.27	K	Cheméo Relay (1.0)
vc	0.417	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
Solubility of N-Hydroxyphthalimide in Binary Acetic Acid + Water Solvent Mixtures at (298.2 to 363.2) K:	https://www.doi.org/10.1021/je600579s
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):	

Legend

hf:	Enthalpy of formation 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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<https://www.chemeo.com/cid/101-745-2/N-hydroxyphthalimide.pdf>

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