6-Nitrobenzimidazole

Inchi: InChI=1S/C7H5N3O2/c11-10(12)5-1-2-6-7(3-5)9-4-8-6/h1-4H,(H,8,9)
InchiKey: XPAZGLFMMUODDK-UHFFFAOYSA-N
Formula: C7H5N3O2
SMILES: O=[N+]([O-])c1ccc2nc[nH]c2c1
Mol. weight [g/mol]: 163.14
CAS: 94-52-0

Physical Properties

Property code	Value	Unit	Source
hf	162.80	kJ/mol	Cheméo Relay (1.0)
hvap	89.92	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	0.989		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
tb	601.94	K	Cheméo Relay (1.0)
tf	481.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

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

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

Latest version available from:
https://www.chemeo.com/cid/106-639-5/6-Nitrobenzimidazole.pdf
Generated by Cheméo on 2026-10-31 06:37:08.509434145 +0000 UTC m=+52341.436271417.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.