

1,3-dihydro-5-nitro-2H-benzimidazol-2-one

Other names:	2H-Benzimidazol-2-one, 1,3-dihydro-5-nitro-
Inchi:	InChI=1S/C7H5N3O3/c11-7-8-5-2-1-4(10(12)13)3-6(5)9-7/h1-3H,(H2,8,9,11)
InchiKey:	DLJZIPVEVJOKHB-UHFFFAOYSA-N
Formula:	C7H5N3O3
SMILES:	O=c1[nH]c2ccc([N+](=O)[O-])cc2[nH]1
Mol. weight [g/mol]:	179.13
CAS:	93-84-5

Physical Properties

Property code	Value	Unit	Source
chs	-3045.50 ± 0.25	kJ/mol	NIST Webbook
hfs	-424.00 ± 0.25	kJ/mol	NIST Webbook
log10ws	-1.79		Crippen Method
logp	-0.199		Crippen Method
mcvol	113.820	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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