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