

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

Other names:	2H-Benzimidazol-2-one, 5-amino-1,3-dihydro-
Inchi:	InChI=1S/C7H7N3O/c8-4-1-2-5-6(3-4)10-7(11)9-5/h1-3H,8H2,(H2,9,10,11)
InchiKey:	BCXSVFBDMPKPT-UHFFFAOYSA-N
Formula:	C7H7N3O
SMILES:	<chem>Nc1ccc2[nH]c(=O)[nH]c2c1</chem>
Mol. weight [g/mol]:	149.15
CAS:	95-23-8

Physical Properties

Property code	Value	Unit	Source
chs	-3337.00 ± 0.65	kJ/mol	NIST Webbook
hfs	-418.00 ± 0.65	kJ/mol	NIST Webbook
log10ws	-0.77		Crippen Method
logp	-0.525		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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