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: BCXSVFBDMPSKPT-UHFFFAOYSA-N
Formula: C7H7N3O
SMILES: Nc1ccc2[nH]c(=O)[nH]c2c1
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/ci990307l

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