N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo

Other names: (2H)Benzimidazol-2-one,1,3-dihydro-5-acetoacetyl-amino-
Inchi: InChI=1S/C11H11N3O3/c1-6(15)4-10(16)12-7-2-3-8-9(5-7)14-11(17)13-8/h2-3,5H,4H2,1
InchiKey: VEMDQCGHZNXORX-UHFFFAOYSA-N
Formula: C11H11N3O3
SMILES: CC(=O)CC(O)=Nc1ccc2nc(O)[nH]c2c1
Mol. weight [g/mol]: 233.22
CAS: 26576-46-5

Physical Properties

Property code	Value	Unit	Source
chs	-5590.00 ± 0.56	kJ/mol	NIST Webbook
hfs	-310.70 ± 0.56	kJ/mol	NIST Webbook
log10ws	-2.31		Crippen Method
logp	1.354		Crippen Method
mcvol	165.880	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26576465&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