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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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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