

2H-Benzimidazol-2-one, 1,3-dihydro-

Other names:	2-Benzimidazolinone 2-Benzimidazolol 2-Benzimidazolone 2(3H)-Benzimidazolone 1,3-Dihydro-2H-benzimidazol-2-one 2-Hydroxybenzimidazole N,N'-(1,2-Phenyleneurea) o-Phenyleneurea Urea, N,N'-(1,2-phenylene)- Benzimidazole-2(3H)-one 2-Oxobenzimidazole 2(3H)-Oxobenzimidazole 2-Hydroxy-1H-benzimidazole NSC 10383 NSC 178108
Inchi:	InChI=1S/C7H6N2O/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H2,8,9,10)
InchiKey:	SILNNFMWIMZVEQ-UHFFFAOYSA-N
Formula:	C7H6N2O
SMILES:	O=c1[nH]c2ccccc2[nH]1
Mol. weight [g/mol]:	134.14
CAS:	615-16-7

Physical Properties

Property code	Value	Unit	Source
chs	-3527.50 ± 3.20	kJ/mol	NIST Webbook
hfs	-85.10 ± 3.20	kJ/mol	NIST Webbook
hsub	126.40 ± 2.40	kJ/mol	NIST Webbook
log10ws	-1.14		Crippen Method
logp	-0.108		Crippen Method
mcvol	96.400	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=C615167&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
hsub: Enthalpy of sublimation 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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