

1H-Benzotriazole, 1-hydroxy-

Other names:	1-benzotriazolol 1-hydroxy-1,2,3-benzotriazole 1-hydroxy-1H-benzotriazole 1-hydroxybenzotriazole 1H-1,2,3-Benzotriazol-1-ol 1H-benzotriazol-1-ol HOBt N-hydroxy-1,2,3-benzotriazole N-hydroxybenzotriazole benzazimidol
Inchi:	InChI=1S/C6H5N3O/c10-9-6-4-2-1-3-5(6)7-8-9/h1-4,10H
InchiKey:	ASOKPJOREAFHNY-UHFFFAOYSA-N
Formula:	C6H5N3O
SMILES:	On1nnc2ccccc21
Mol. weight [g/mol]:	135.12
CAS:	2592-95-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	0.187		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
tf	424.26	K	Thermodynamic Functions for Solubility of 1-Hydroxybenzotriazole in Sixteen Solvents at Temperatures from (278.15 to 313.15) K and Mixing Property of Mixtures

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2592952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

**Thermodynamic Functions for
Solubility of 1-Hydroxybenzotriazole in
Sixteen Solvents at Temperatures from
(278.15 to 313.15) K and Mixing
Property of Mixtures:**

<https://www.doi.org/10.1021/acs.jced.7b00316>

<http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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