

2-Benzimidazolylurea

Other names:	Urea, 1H-benzimidazol-2-yl- Benzimidazol-2-ylurea Urea, (2-benzimidazolyl)- 2-Benzimidazoleurea 2-Ureidobenzimidazole Urea, benzimidazol-2-yl-
Inchi:	InChI=1S/C8H8N4O/c9-7(13)12-8-10-5-3-1-2-4-6(5)11-8/h1-4H,(H4,9,10,11,12,13)
InchiKey:	LNYZEFQMIURYEI-UHFFFAOYSA-N
Formula:	C8H8N4O
SMILES:	NC(=O)Nc1nc2cccc2[nH]1
Mol. weight [g/mol]:	176.18
CAS:	24370-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	0.572		Crippen Method
mcvol	126.150	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24370250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	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

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