

N-Benzoylimidazole

Other names:	1-Benzoylimidazole 1H-Imidazole, 1-benzoyl-
Inchi:	InChI=1S/C10H8N2O/c13-10(12-7-6-11-8-12)9-4-2-1-3-5-9/h1-8H
InchiKey:	JEGIFBGJZPYMJS-UHFFFAOYSA-N
Formula:	C10H8N2O
SMILES:	O=C(c1cccc1)n1ccnc1
Mol. weight [g/mol]:	172.18
CAS:	10364-94-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.572		Crippen Method
mvol	130.070	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10364940&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

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