

2-Benzamido-5-nitrothiazole

Other names:	N-(5-nitro-2-thiazolyl)benzamide
Inchi:	InChI=1S/C10H7N3O3S/c14-9(7-4-2-1-3-5-7)12-10-11-6-8(17-10)13(15)16/h1-6H,(H,11,
InchiKey:	TYUHMMUUMWZPDB-UHFFFAOYSA-N
Formula:	C10H7N3O3S
SMILES:	O=C(Nc1ncc([N+](=O)[O-])s1)c1ccccc1
Mol. weight [g/mol]:	249.25
CAS:	64398-84-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.304		Crippen Method
mcvol	163.840	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64398841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/45-529-5/2-Benzamido-5-nitrothiazole.pdf>

Generated by Cheméo on 2024-05-19 17:33:48.705599148 +0000 UTC m=+18429277.626176464.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.