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.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