

Imidazole-4-carboxamide, n-butyl-5-nitro-

Inchi: InChI=1S/C8H12N4O3/c1-2-3-4-9-8(13)6-7(12(14)15)11-5-10-6/h5H,2-4H2,1H3,(H,9,13)
InchiKey: ZFDNSAMIBQTEDS-UHFFFAOYSA-N
Formula: C8H12N4O3
SMILES: CCCCNC(=O)c1nc[nH]c1[N+](=O)[O-]
Mol. weight [g/mol]: 212.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	0.366		Crippen Method
mcvol	153.050	ml/mol	McGowan Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010470&Units=SI>

Legend

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

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