

Imidazole, 4-(4-methylpiperidinocarbonyl)-5-nitro-

Inchi: InChI=1S/C10H14N4O3/c1-7-2-4-13(5-3-7)10(15)8-9(14(16)17)12-6-11-8/h6-7H,2-5H2,1
InchiKey: CORMEMYMWIPHDW-UHFFFAOYSA-N
Formula: C10H14N4O3
SMILES: CC1CCN(C(=O)c2nc[nH]c2[N+](=O)[O-])CC1
Mol. weight [g/mol]: 238.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	0.708		Crippen Method
mcvol	170.370	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008684&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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