Imidazole, 4-morpholinocarbonyl-5-nitro-

Inchi: InChI=1S/C8H10N4O4/c13-8(11-1-3-16-4-2-11)6-7(12(14)15)10-5-9-6/h5H,1-4H2,(H,9,1
InchiKey: KXIXGAZCTMEOTP-UHFFFAOYSA-N
Formula: C8H10N4O4
SMILES: O=C(c1nc[nH]c1[N+](=O)[O-])N1CCOCC1
Mol. weight [g/mol]: 226.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	-0.692		Crippen Method
mcvol	148.060	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008241&Units=SI

Legend

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