

Dimetridazole

Other names:	1,2-Dimethyl-5-nitro-1H-imidazole 1,2-dimethyl-5-nitroimidazole 1H-Imidazole, 1,2-dimethyl-5-nitro- 5-Nitro-1,2-dimethylimidazole 8595 R.P. Dimetridazol Dimetrizadole Emtryl Emtrylvet Emtrymix Imidazole, 1,2-dimethyl-5-nitro- NSC 226253 RP 8595 Unizole Soluble
Inchi:	InChI=1S/C5H7N3O2/c1-4-6-3-5(7(4)2)8(9)10/h3H,1-2H3
InchiKey:	IBXPYPUJPLLOIN-UHFFFAOYSA-N
Formula:	C5H7N3O2
SMILES:	<chem>Cc1ncc([N+](=O)[O-])n1C</chem>
Mol. weight [g/mol]:	141.13
CAS:	551-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	0.637		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
rinpole	1353.00		NIST Webbook
rinpole	1353.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C551928&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Investigation on molecular interactions of antibiotics in alcohols using McGowan Method: Thermodynamic studies at different temperatures: <https://www.doi.org/10.1016/j.jct.2016.09.037>
<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
rinpol: Non-polar retention indices

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