

AMETAZOLE

Other names:	1H-Pyrazole-3-ethanamine 3-(2-Aminoethyl)pyrazole 3-Aminoethylpyrazole Ametazole Pyrazole, 3-(2-aminoethyl)-
Inchi:	InChI=1S/C5H9N3/c6-3-1-5-2-4-7-8-5/h2,4H,1,3,6H2,(H,7,8)
InchiKey:	JXDFAQONERDKSS-UHFFFAOYSA-N
Formula:	C5H9N3
SMILES:	NCCc1cc[nH]n1
Mol. weight [g/mol]:	111.15

Physical Properties

Property code	Value	Unit	Source
logp	-0.571		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
rinpol	1390.00		NIST Webbook

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105204&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/80-796-0/AMETAZOLE.pdf>

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