

2-AMINOPURINE

Other names:	1H-Purin-2-amine Purine, 2-amino- SQ 22,451 SQ 22451
Inchi:	InChI=1S/C5H5N5/c6-5-7-1-3-4(10-5)9-2-8-3/h1-2H,(H3,6,7,8,9,10)
InchiKey:	MWBWWFOAEOYUST-UHFFFAOYSA-N
Formula:	C5H5N5
SMILES:	<chem>Nc1ncc2nc[nH]c2n1</chem>
Mol. weight [g/mol]:	135.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Cheméo Relay (1.0)
logp	-0.547		Crippen Method
mcvol	92.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C452062&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

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