

1-Amino-4-methylpiperazine

Other names:	1-Piperazinamine, 4-methyl- 4-methylpiperazin-1-amine
Inchi:	InChI=1S/C5H13N3/c1-7-2-4-8(6)5-3-7/h2-6H2,1H3
InchiKey:	RJWLLQWLBMJCFD-UHFFFAOYSA-N
Formula:	C5H13N3
SMILES:	CN1CCN(N)CC1
Mol. weight [g/mol]:	115.18
CAS:	6928-85-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.63		Crippen Method
logp	-0.892		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
tb	446.70	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6928854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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