

2,5-Diaza-5-methylcycloheptanone

Inchi:	InChI=1S/C6H12N2O/c1-8-4-2-6(9)7-3-5-8/h2-5H2,1H3,(H,7,9)
InchiKey:	FZYSZYWKHFCLSF-UHFFFAOYSA-N
Formula:	C6H12N2O
SMILES:	CN1CCNC(=O)CC1
Mol. weight [g/mol]:	128.17
CAS:	5441-40-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.24		Crippen Method
logp	-0.562		Crippen Method
mcvol	106.070	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5441407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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