

Pyrazine, 2-(2-pyrrylmethyl)-3,6-dimethyl

Inchi:	InChI=1S/C11H13N3/c1-8-7-13-9(2)11(14-8)6-10-4-3-5-12-10/h3-5,7,12H,6H2,1-2H3
InchiKey:	GLPZVZHBMYAUNA-UHFFFAOYSA-N
Formula:	C11H13N3
SMILES:	Cc1cnc(C)c(Cc2ccc[nH]2)n1
Mol. weight [g/mol]:	187.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	1.530		Crippen Method
mcvol	152.570	ml/mol	McGowan Method
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R87893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	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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<https://www.chemeo.com/cid/94-583-1/Pyrazine-2-2-pyrrylmethyl-3-6-dimethyl.pdf>

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