

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

Other names:	3-(2-furfuryl)-2,5-dimethylpyrazine 3-Furfuryl-2,5-dimethyl pyrazine
Inchi:	InChI=1S/C11H12N2O/c1-8-7-12-9(2)11(13-8)6-10-4-3-5-14-10/h3-5,7H,6H2,1-2H3
InchiKey:	QJSGHKNKGABEQR-UHFFFAOYSA-N
Formula:	C11H12N2O
SMILES:	<chem>Cc1cnc(C)c(Cc2ccco2)n1</chem>
Mol. weight [g/mol]:	188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.79		Crippen Method
logp	2.277		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1409.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1413.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R87857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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