

Pyrazine, 2-(2-furfuryl)-6-methyl

Other names:	2-(2-furfuryl)-6-methylpyrazine
Inchi:	InChI=1S/C10H10N2O/c1-8-6-11-7-9(12-8)5-10-3-2-4-13-10/h2-4,6-7H,5H2,1H3
InchiKey:	GODMWVHOELDUKF-UHFFFAOYSA-N
Formula:	C10H10N2O
SMILES:	Cc1cncc(Cc2ccco2)n1
Mol. weight [g/mol]:	174.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	1.969		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
rinpol	1361.00		NIST Webbook
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rinpol	1361.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R87875&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
rinpol:	Non-polar retention indices

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