2-(2'-furyl)-6-methylpyrazine

Other names: 2-(2-Furyl)-6-methylpyrazine
Inchi: InChI=1S/C9H8N2O/c1-7-5-10-6-8(11-7)9-3-2-4-12-9/h2-6H,1H3
InchiKey: HEVHVDDCDVZQTL-UHFFFAOYSA-N
Formula: C9H8N2O
SMILES: Cc1cncc(-c2ccco2)n1
Mol. weight [g/mol]: 160.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.82		Crippen Method
logp	2.045		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
rinpol	1381.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1381.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R236552&Units=SI

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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