2-(2-Furyl)-5,6-dimethylpyrazine

Inchi: InChI=1S/C10H10N2O/c1-7-8(2)12-9(6-11-7)10-4-3-5-13-10/h3-6H,1-2H3
InchiKey: ITNKCJNTYFLMPS-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: Cc1ncc(-c2ccco2)nc1C
Mol. weight [g/mol]: 174.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.29		Crippen Method
logp	2.353		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
rinpol	1452.00		NIST Webbook

Sources

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=R323245&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices