2-Furyl pyrazine

Other names: 2-(2'-Furyl)pyrazine
2-(2-Furyl)pyrazine
(2'-Furyl)pyrazine
Inchi: InChI=1S/C8H6N2O/c1-2-8(11-5-1)7-6-9-3-4-10-7/h1-6H
InchiKey: XAZULAQXFJZQTJ-UHFFFAOYSA-N
Formula: C8H6N2O
SMILES: c1coc(-c2cnccn2)c1
Mol. weight [g/mol]: 146.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	1.737		Crippen Method
mcvol	106.190	ml/mol	McGowan Method
rinpol	1288.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1255.00		NIST Webbook
ripol	2022.00		NIST Webbook
ripol	2022.00		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=R87982&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
ripol:	Polar retention indices