

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:	<chem>c1coc(-c2cnccn2)c1</chem>
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/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/18-961-5/2-Furyl-pyrazine.pdf>

Generated by Cheméo on 2024-05-02 02:40:03.10824875 +0000 UTC m=+16906852.028826066.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.