

Pyrazine, ethoxy-

Other names:	2-Ethoxypyrazine 3-Ethoxypyrazine Ethoxypyrazine Pyrazine, 2-ethoxy-
Inchi:	InChI=1S/C6H8N2O/c1-2-9-6-5-7-3-4-8-6/h3-5H,2H2,1H3
InchiKey:	ATIUKJHILQVQLE-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	CCOc1cnccn1
Mol. weight [g/mol]:	124.14
CAS:	38028-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.875		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
ripol	1348.00		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=C38028670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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.chemeo.com/cid/10-958-7/Pyrazine-ethoxy.pdf>

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