

Pyrazine, 2-methoxy-3-methyl-

Other names:	2-Methoxy-3-methylpyrazine 2-Methyl-3-methoxypyrazine Methoxymethylpyrazine Pyrazine, 2-methyl-3-methoxy
Inchi:	InChI=1S/C6H8N2O/c1-5-6(9-2)8-4-3-7-5/h3-4H,1-2H3
InchiKey:	VKJIAEQRKBQLLA-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	COc1nccnc1C
Mol. weight [g/mol]:	124.14
CAS:	2847-30-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	0.794		Crippen Method
mcpvol	97.470	ml/mol	McGowan Method
ripol	954.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1339.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2847305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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