

Pyrazine, 2-ethoxy-5-methyl-

Other names:	Pyrazine, 5-ethoxy-2-methyl 2-Ethoxy-5-methylpyrazine
Inchi:	InChI=1S/C7H10N2O/c1-3-10-7-5-8-6(2)4-9-7/h4-5H,3H2,1-2H3
InchiKey:	MGDMTRSONRZXOH-UHFFFAOYSA-N
Formula:	C7H10N2O
SMILES:	CCOc1cnc(C)cn1
Mol. weight [g/mol]:	138.17
CAS:	67845-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.184		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1418.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67845345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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