

Pyrazine, 3-ethoxy-2-pentyl

Other names:	Pyrazine, 2-ethoxy-3-pentyl
Inchi:	InChI=1S/C11H18N2O/c1-3-5-6-7-10-11(14-4-2)13-9-8-12-10/h8-9H,3-7H2,1-2H3
InchiKey:	ZTFRROZFJBQMHI-UHFFFAOYSA-N
Formula:	C11H18N2O
SMILES:	CCCCCc1nccnc1OCC
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.608		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1691.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R43659&Units=SI
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

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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