

2-methyl-3-octylpyrazine

Other names:	Pyrazine, 2-methyl-3-octyl
Inchi:	InChI=1S/C13H22N2/c1-3-4-5-6-7-8-9-13-12(2)14-10-11-15-13/h10-11H,3-9H2,1-2H3
InchiKey:	TWJYEPWTOVCD SJ-UHFFFAOYSA-N
Formula:	C13H22N2
SMILES:	CCCCCCCCc1nccnc1C
Mol. weight [g/mol]:	206.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	3.688		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1956.00		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=R38420&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

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