

Octylpyrazine

Other names:	Pyrazine, octyl
Inchi:	InChI=1S/C12H20N2/c1-2-3-4-5-6-7-8-12-11-13-9-10-14-12/h9-11H,2-8H2,1H3
InchiKey:	VEIAXROYVVCIER-UHFFFAOYSA-N
Formula:	C12H20N2
SMILES:	CCCCCCCCc1cnccn1
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	3.380		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
ripol	1845.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38797&Units=SI

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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