

Pyrazine, 2,3-dimethyl-5-pentyl

Other names:	2,3-dimethyl-5-pentylpyrazine
Inchi:	InChI=1S/C11H18N2/c1-4-5-6-7-11-8-12-9(2)10(3)13-11/h8H,4-7H2,1-3H3
InchiKey:	VKYMJNLWOOCXDZ-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CCCCCc1cnc(C)c(C)n1
Mol. weight [g/mol]:	178.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.826		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1352.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1283.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R38256&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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