

Pyrazine, 3,5-dimethyl-2-propyl-

Other names:	2,6-Dimethyl-3-propylpyrazine Pyrazine, 2,6-dimethyl-3-propyl- 3,5-Dimethyl-2-propylpyrazine 2,6-Dimethyl-3-pyropylpyrazine
Inchi:	InChI=1S/C9H14N2/c1-4-5-9-8(3)11-7(2)6-10-9/h6H,4-5H2,1-3H3
InchiKey:	UTRAUCDSVCDVIW-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCc1ncc(C)nc1C
Mol. weight [g/mol]:	150.22
CAS:	32350-16-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.046		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1151.00		NIST Webbook
ripol	1493.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32350166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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