

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

Other names:	2-Propyl-3,6-dimethylpyrazine 2,5-Dimethyl-3-propylpyrazine 3,6-Dimethyl-2-propylpyrazine 2,5-Dimethyl-3-propylpyrazine
Inchi:	InChI=1S/C9H14N2/c1-4-5-9-8(3)10-6-7(2)11-9/h6H,4-5H2,1-3H3
InchiKey:	ARRSOXMGLBJPNV-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCc1nc(C)cnc1C
Mol. weight [g/mol]:	150.22
CAS:	18433-97-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.046		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
ripol	1141.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		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=C18433971&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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