

Pyrazine, 2,6-dimethyl-

Other names:	2,6-Dimethylpyrazine 3,5-Dimethylpyrazine
Inchi:	InChI=1S/C6H8N2/c1-5-3-7-4-6(2)8-5/h3-4H,1-2H3
InchiKey:	HJFZAYHYIWGLNL-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	Cc1cncc(C)n1
Mol. weight [g/mol]:	108.14
CAS:	108-50-9

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.093		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	888.90		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	906.00		NIST Webbook
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Sources

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McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108509&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature

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