

Pyrazine, 2,3-diethyl-5-methyl-

Other names:	2-Methyl-5,6-diethylpyrazine 2,3-Diethyl-5-methylpyrazine 5-Methyl-2,3-diethylpyrazine 2,3-Diethyl-6-methylpyrazine
Inchi:	InChI=1S/C9H14N2/c1-4-8-9(5-2)11-7(3)6-10-8/h6H,4-5H2,1-3H3
InchiKey:	PSINWXIDJYEXLO-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCc1ncc(C)nc1CC
Mol. weight [g/mol]:	150.22
CAS:	18138-04-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	1.910		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1151.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1155.00		NIST Webbook

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ripol	1505.00	NIST Webbook

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ripol	1483.00	NIST Webbook
ripol	1492.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1494.00	NIST Webbook
ripol	1482.00	NIST Webbook
ripol	1484.00	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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=C18138040&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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