

2,3,5-Trimethyl-6-ethylpyrazine

Other names:	2-Ethyl-3,5,6-trimethylpyrazine 6-Ethyl-2,3,5-trimethylpyrazine Pyrazine, ethyltrimethyl
Inchi:	InChI=1S/C9H14N2/c1-5-9-8(4)10-6(2)7(3)11-9/h5H2,1-4H3
InchiKey:	FPOLJKZKOKXIFE-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCc1nc(C)c(C)nc1C
Mol. weight [g/mol]:	150.22
CAS:	17398-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	1.964		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
ripol	1127.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1155.50		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1169.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1521.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C17398162&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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