

Pyrazine, 2-ethyl-3-(methylthio)-

Other names:	2-(Methylthio)-3-ethylpyrazine 2-Ethyl-3-methylthiopyrazine 3-Ethyl-2-(methylthio)pyrazine Pyrazine, 3-ethyl-2-(methylthio)
Inchi:	InChI=1S/C7H10N2S/c1-3-6-7(10-2)9-5-4-8-6/h4-5H,3H2,1-2H3
InchiKey:	XYHPPOMSLGJAAM-UHFFFAOYSA-N
Formula:	C7H10N2S
SMILES:	CCc1nccnc1SC
Mol. weight [g/mol]:	154.23
CAS:	72987-62-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.761		Crippen Method
mcpvol	122.040	ml/mol	McGowan Method
ripol	1267.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1695.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72987623&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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