

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

Other names:	2-Methyl-3-(methylthio)pyrazine 2-Methyl-3-methylmercaptopyrazine 2-Methylthio-3-methylpyrazine 3-Methyl-2-methylthiopyrazine Methylmethylthiopyrazine 2-Methylmercapto-3-methylpyrazine
Inchi:	InChI=1S/C6H8N2S/c1-5-6(9-2)8-4-3-7-5/h3-4H,1-2H3
InchiKey:	PPFFGVGWFKTHX-UHFFFAOYSA-N
Formula:	C6H8N2S
SMILES:	CSc1nccnc1C
Mol. weight [g/mol]:	140.21
CAS:	2882-20-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.507		Crippen Method
mcpvol	107.950	ml/mol	McGowan Method
ripol	1145.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1616.00		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=C2882204&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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