

Pyrazine, (ethylthio)

Other names:	(Ethylthio)pyrazine
Inchi:	InChI=1S/C6H8N2S/c1-2-9-6-5-7-3-4-8-6/h3-5H,2H2,1H3
InchiKey:	XOBSTMSWRISSIN-UHFFFAOYSA-N
Formula:	C6H8N2S
SMILES:	CCSc1cnccn1
Mol. weight [g/mol]:	140.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	1.589		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
ripol	1635.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R36387&Units=SI
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

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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