Pyrazine, (methylthio)-

Other names:	2-(Methylsulfanyl)pyrazine
	(Methylthio)pyrazine
	Methyl pyrazinyl sulfide
Inchi:	InChI=1S/C5H6N2S/c1-8-5-4-6-2-3-7-5/h2-4H,1H3
InchiKey:	KBPBOWBQRUXMFV-UHFFFAOYSA-N
Formula:	C5H6N2S
SMILES:	CSc1cnccn1
Mol. weight [g/mol]:	126.18
CAS:	21948-70-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.198		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
ripol	1600.00		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=C21948709&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