

[(methylthio)propyl]pyrazine

Inchi: InChI=1S/C8H12N2S/c1-11-6-2-3-8-7-9-4-5-10-8/h4-5,7H,2-3,6H2,1H3
InchiKey: QWZQTCWSFURDKY-UHFFFAOYSA-N
Formula: C8H12N2S
SMILES: CSCCCc1cnccn1
Mol. weight [g/mol]: 168.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	1.772		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1386.00		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=R221575&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

Latest version available from:

<https://www.chemeo.com/cid/13-300-3/methylthio-propyl-pyrazine.pdf>

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