

Pyrazine, 2-methylthio-3-propyl

Inchi: InChI=1S/C8H12N2S/c1-3-4-7-8(11-2)10-6-5-9-7/h5-6H,3-4H2,1-2H3
InchiKey: BEHCKYZOZCUEQ-UHFFFAOYSA-N
Formula: C8H12N2S
SMILES: CCCc1nccnc1SC
Mol. weight [g/mol]: 168.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	2.151		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1764.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=R43560&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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