

2,3-dimethyl-5-[(methylthio)propyl]pyrazine

Inchi: InChI=1S/C10H16N2S/c1-8-9(2)12-10(7-11-8)5-4-6-13-3/h7H,4-6H2,1-3H3
InchiKey: HYLJMJNFTZYRKA-UHFFFAOYSA-N
Formula: C10H16N2S
SMILES: CSCCCc1cnc(C)c(C)n1
Mol. weight [g/mol]: 196.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.389		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2260.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U366012&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/94-535-4/2-3-dimethyl-5-methylthio-propyl-pyrazine.pdf>

Generated by Cheméo on 2024-04-26 17:43:17.976628349 +0000 UTC m=+16442646.897205661.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.