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/ci990307l
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