Pyrazine, 3-methyl-5-(1-methylbutyl)-2-(methylthio)

Inchi: InChI=1S/C11H18N2S/c1-5-6-8(2)10-7-12-11(14-4)9(3)13-10/h7-8H,5-6H2,1-4H3
InchiKey: JQDIOIIJMLKYQF-UHFFFAOYSA-N
Formula: C11H18N2S
SMILES: CCCC(C)c1cnc(SC)c(C)n1
Mol. weight [g/mol]: 210.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.411		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R217724&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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