3-methyl-5-(2-methylpentyl)-2-(methylthio)pyrazin

Other names: Pyrazine, 3-methyl-5-(2-methylpentyl)-2-(methylthio)
Inchi: InChI=1S/C12H20N2S/c1-5-6-9(2)7-11-8-13-12(15-4)10(3)14-11/h8-9H,5-7H2,1-4H3
InchiKey: LJKPXYGPGYYPSW-UHFFFAOYSA-N
Formula: C12H20N2S
SMILES: CCCC(C)Cc1cnc(SC)c(C)n1
Mol. weight [g/mol]: 224.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.486		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
ripol	2008.00		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=R38569&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