

Pyrazine, 2,3-dimethyl-5-(2-methylpentyl)

Other names: 2,3-dimethyl-5-(2-methylpentyl)pyrazine
Inchi: InChI=1S/C12H20N2/c1-5-6-9(2)7-12-8-13-10(3)11(4)14-12/h8-9H,5-7H2,1-4H3
InchiKey: HPVPVLBZELBDEX-UHFFFAOYSA-N
Formula: C12H20N2
SMILES: CCCC(C)Cc1cnc(C)c(C)n1
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	3.072		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1710.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38224&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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