2,3,5-TRIMETHYL-6-(2-METHYLBUTYL)PYRAZINE

Other names: 2-(2-methylbutyl)-3,5,6-trimethylpyrazine
Pyrazine, 3,5,6-trimethyl-2-(2-methylbutyl)
Inchi: InChI=1S/C12H20N2/c1-6-8(2)7-12-11(5)13-9(3)10(4)14-12/h8H,6-7H2,1-5H3
InchiKey: HBNTYRSZFUEIEX-UHFFFAOYSA-N
Formula: C12H20N2
SMILES: CCC(C)Cc1nc(C)c(C)nc1C
Mol. weight [g/mol]: 192.31

Physical Properties

Property code	Value	Unit	Source
logp	2.990		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1363.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1661.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18482809&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices