

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]:	192.30
CAS:	18482-80-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	2.990		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1363.00		NIST Webbook
ripol	1661.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18482809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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