

2,3,5-Trimethyl-6-butylpyrazine

Other names:	2-Butyl-3,5,6-trimethylpyrazine Trimethylbutylpyrazine Butyltrimethylpyrazine Pyrazine, butyltrimethyl-
Inchi:	InChI=1S/C11H18N2/c1-5-6-7-11-10(4)12-8(2)9(3)13-11/h5-7H2,1-4H3
InchiKey:	LHDGCKPZCAXIBB-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CCCCc1nc(C)c(C)nc1C
Mol. weight [g/mol]:	178.27
CAS:	10132-38-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	2.744		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinsol	1260.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10132384&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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