

2,6-Bis(2-methylpropyl)pyrazine

Other names:	2,6-Diisobutylpyrazine
Inchi:	InChI=1S/C12H20N2/c1-9(2)5-11-7-13-8-12(14-11)6-10(3)4/h7-10H,5-6H2,1-4H3
InchiKey:	WEKSWAFOTVHVQR-UHFFFAOYSA-N
Formula:	C12H20N2
SMILES:	CC(C)Cc1cncc(CC(C)C)n1
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.874		Crippen Method
mcvol	176.140	ml/mol	McGowan Method

Sources

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=U108600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/49-570-5/2-6-Bis-2-methylpropyl-pyrazine.pdf>

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