

3-methyl-5-(2-methylpentyl)-2-(methylthio)pyrazine

Other names:	Pyrazine, 3-methyl-5-(2-methylpentyl)-2-(methylthio)
Inchi:	InChI=1S/C12H20N2S/c1-5-6-9(2)7-11-8-13-12(15-4)10(3)14-11/h8-9H,5-7H2,1-4H3
InchiKey:	LJKPXYGPGYYPSW-UHFFFAOYSA-N
Formula:	C12H20N2S
SMILES:	CCCC(C)Cc1cnc(SC)c(C)n1
Mol. weight [g/mol]:	224.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.486		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
ripol	2008.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R38569&Units=SI

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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