2,3-Dimethyl-5-isopentylpyrazine

Other names:	5-Isopentyl-2,3-dimethylpyrazine
	Pyrazine, 2,3-dimethyl-5-(3-methylbutyl)
Inchi:	InChI=1S/C11H18N2/c1-8(2)5-6-11-7-12-9(3)10(4)13-11/h7-8H,5-6H2,1-4H3
InchiKey:	OGUJUYCURMHXHG-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	Cc1ncc(CCC(C)C)nc1C
Mol. weight [g/mol]:	178.27
CAS:	18450-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.682		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1332.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1646.00		NIST Webbook

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=C18450016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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