2-Isoamyl-6-methylpyrazine

Other names:	2-Methyl-6-isopentylpyrazine
	6-Methyl-2-(3-methylbutyl)-pyrazine
	Pyrazine, 2-methyl-6-(3-methylbutyl)-
	2-Isopentyl-6-methylpyrazine
Inchi:	InChI=1S/C10H16N2/c1-8(2)4-5-10-7-11-6-9(3)12-10/h6-8H,4-5H2,1-3H3
InchiKey:	OESNKUIGZMJYKH-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	Cc1cncc(CCC(C)C)n1
Mol. weight [g/mol]:	164.25
CAS:	91010-41-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	2.374		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1248.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1249.00		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=C91010412&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