2-Isoamylpyrazine

Other names:	3-Methylbutylpyrazine
	Isopentyl pyrazine
	Pyrazine, (3-methylbutyl)
Inchi:	InChI=1S/C9H14N2/c1-8(2)3-4-9-7-10-5-6-11-9/h5-8H,3-4H2,1-2H3
InchiKey:	ILKAUWPPPOYQHF-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CC(C)CCc1cnccn1
Mol. weight [g/mol]:	150.22
CAS:	40790-22-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.065		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1156.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1157.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1530.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40790225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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