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

Other names:	Pyrazine, 2-chloro-3-methyl-5-(2-methylpentyl)
Inchi:	InChI=1S/C11H17ClN2/c1-4-5-8(2)6-10-7-13-11(12)9(3)14-10/h7-8H,4-6H2,1-3H3
InchiKey:	YOZRPCPCVYSOEH-UHFFFAOYSA-N
Formula:	C11H17ClN2
SMILES:	CCCC(C)Cc1cnc(Cl)c(C)n1
Mol. weight [g/mol]:	212.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	3.417		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rinpol	1456.00		NIST Webbook
ripol	1789.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38288&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

Latest version available from:

https://www.chemeo.com/cid/41-156-3/2-chloro-3-methyl-5-2-methylpentyl-pyrazine.pdf

Generated by Cheméo on 2024-10-12 06:08:13.094415836 +0000 UTC m=+3294155.731385086.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.