

Pyrazine, 2-chloro-3-methyl-5-(1-methylethyl)

Other names: 2-chloro-5-isopropyl-3-methylpyrazine
Inchi: InChI=1S/C8H11ClN2/c1-5(2)7-4-10-8(9)6(3)11-7/h4-5H,1-3H3
InchiKey: LUYCBAHXNPHQJE-UHFFFAOYSA-N
Formula: C8H11ClN2
SMILES: Cc1nc(C(C)C)cnc1Cl
Mol. weight [g/mol]: 170.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.562		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
ripol	1505.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38309&Units=SI>
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>

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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