

2,5-Dimethyl-3-isopropylpyrazine

Inchi: InChI=1S/C9H14N2/c1-6(2)9-8(4)10-5-7(3)11-9/h5-6H,1-4H3
InchiKey: NJTFLPVGROFSPU-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: Cc1cnc(C)c(C(C)C)n1
Mol. weight [g/mol]: 150.22
CAS: 13610-20-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	2.217		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpola	1177.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13610203&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpola: Non-polar retention indices

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