2-(1-Methylethenyl)-5-(1-methylethyl)pyrazine

Inchi: InChI=1S/C10H14N2/c1-7(2)9-5-12-10(6-11-9)8(3)4/h5-6,8H,1H2,2-4H3
InchiKey: RVKVUYGBDYOOJD-UHFFFAOYSA-N
Formula: C10H14N2
SMILES: C=C(C)c1cnc(C(C)C)cn1
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.633		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook

Sources

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=R412810&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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