

2-Methyl-5-isopropyl furan

Inchi: InChI=1S/C8H12O/c1-6(2)8-5-4-7(3)9-8/h4-6H,1-3H3
InchiKey: JYOVNNBTWWYRGU-UHFFFAOYSA-N
Formula: C8H12O
SMILES: Cc1ccc(C(C)C)o1
Mol. weight [g/mol]: 124.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.87		Crippen Method
logp	2.711		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
rinpola	933.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R325805&Units=SI>

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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