

5-(Furan-3-yl)-2-methylpent-1-en-3-ol

Inchi: InChI=1S/C10H14O2/c1-8(2)10(11)4-3-9-5-6-12-7-9/h5-7,10-11H,1,3-4H2,2H3
InchiKey: YIVMCXYIUTUOOZ-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: C=C(C)C(O)CCc1ccoc1
Mol. weight [g/mol]: 166.22
CAS: 72075-28-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	2.149		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1277.70		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C72075286&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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