

beta-Methylcinnamyl alcohol

Inchi: InChI=1S/C10H12O/c1-9(7-8-11)10-5-3-2-4-6-10/h2-7,11H,8H2,1H3/b9-7+
InchiKey: GASLYRXUZSPLGV-VQHVLOKHSA-N
Formula: C10H12O
SMILES: CC(=CC(O))c1ccccc1
Mol. weight [g/mol]: 148.20
CAS: 1504-54-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	2.520		Crippen Method
mcvol	127.420	ml/mol	McGowan Method
rinpol	1365.00		NIST Webbook
ripol	2283.00		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=C1504547&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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