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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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https://www.chemeo.com/cid/44-039-0/beta-Methylcinnamyl-alcohol.pdf

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