

2,6-Dimethyl-1,6-heptadien-4-ol

Inchi:	InChI=1S/C9H16O/c1-7(2)5-9(10)6-8(3)4/h9-10H,1,3,5-6H2,2,4H3
InchiKey:	BUCLVUABDUWMHW-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	C=C(C)CC([O])CC(=C)C
Mol. weight [g/mol]:	140.22
CAS:	29765-76-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.718		Crippen Method
mcvol	132.790	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C29765762&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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