

2-acetoxymethylenecyclohexene

Inchi: InChI=1S/C17H22O3/c1-11-6-5-7-12(2)10-16-15(9-8-11)13(3)17(20-16)19-14(4)18/h7-8H
InchiKey: DDIISBOPYNGSCV-OHJCXFAUSA-N
Formula: C₁₇H₂₂O₃
SMILES: CC(=O)Oc1cc2c(c1C)CC=C(C)CCC=C(C)C2
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.71		Crippen Method
logp	4.285		Crippen Method
mcvol	224.780	ml/mol	McGowan Method
rinpol	1884.00		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=R303850&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/12-088-1/2-acetoxymethylenecyclohexene.pdf>

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