

Methyl strictate

Inchi: InChI=1S/C21H28O3/c1-16-8-9-17(2)21(3,13-10-18-11-14-24-15-18)12-6-5-7-19(16)20(2)
InchiKey: UQBKEKGILPGMIT-VLNUDNINSA-N
Formula: C₂₁H₂₈O₃
SMILES: C=C1CCC(C)C(C)(CCc2ccoc2)CC=CC=C1C(=O)OC
Mol. weight [g/mol]: 328.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.12		Crippen Method
logp	5.250		Crippen Method
mcvol	276.840	ml/mol	McGowan Method
rinpole	2430.00		NIST Webbook
rinpole	2430.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R626589&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/96-358-9/Methyl-strictate.pdf>

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