Cyclopenta[c]pyran-4-ylmethyl 3-methylbutanoate

Inchi: InChI=1S/C14H16O3/c1-10(2)6-14(15)17-9-12-8-16-7-11-4-3-5-13(11)12/h3-5,7-8,10H,6

InchiKey: AZDUKOUQTRSWCE-UHFFFAOYSA-N

Formula: C14H16O3

SMILES: CC(C)CC(=O)OCc1cocc2cccc1-2

Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	3.474		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	1783.10		NIST Webbook
rinpol	1783.10		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=U412865&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.