5-(3,5-dimethylheptanyl)-3-methyl-2H-pyran-2-one diastereomer 2

Inchi: InChI=1S/C15H24O2/c1-5-11(2)10-12(3)6-8-14-9-7-13(4)15(16)17-14/h7,9,11-12H,5-6,8

InchiKey: NEMOHEQHTVPJLI-UHFFFAOYSA-N

Formula: C15H24O2

SMILES: CCC(C)CC(C)CCc1ccc(C)c(=O)o1

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	3.953		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook
ripol	2592.00		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=R494807&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

ripol: Polar retention indices

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