

5-(2,4-dimethylheptanyl)-3-methyl-2H-pyran-2-one

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

Formula: C15H24O2
SMILES: CCCC(C)CC(C)Cc1ccc(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	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
ripol	2515.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R494758&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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