5-(2,5-dimethylheptanyl)-3-methyl-2H-pyran-2-one diastereomer 1

Inchi: InChI=1S/C15H24O2/c1-5-11(2)6-7-12(3)10-14-9-8-13(4)15(16)17-14/h8-9,11-12H,5-7,1

InchiKey: XBJHSMUZOJJYBO-UHFFFAOYSA-N

Formula: C15H24O2

SMILES: CCC(C)CCC(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	1836.00		NIST Webbook
ripol	2552.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R494763&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