

5-(2-ethyl,5-methylheptanyl)-3-methyl-2H-pyran-2-

Inchi: InChI=1S/C16H26O2/c1-5-12(3)7-9-14(6-2)11-15-10-8-13(4)16(17)18-15/h8,10,12,14H,5
InchiKey: RFRSCTCURWTACN-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CCC(C)CCC(CC)Cc1ccc(C)c(=O)o1
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	4.343		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
rinpol	1809.00		NIST Webbook
rinpol	1809.00		NIST Webbook
ripol	2498.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R494783&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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