Amyl furfurylacrylate

Inchi: InChI=1S/C12H16O3/c1-2-3-4-9-15-12(13)8-7-11-6-5-10-14-11/h5-8,10H,2-4,9H2,1H3/b
InchiKey: XMIDBHIKAVTGQN-BQYQJAHWSA-N
Formula: C12H16O3
SMILES: CCCCCOC(=O)C=Cc1ccco1
Mol. weight [g/mol]: 208.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.40		Crippen Method
logp	3.026		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
rinpol	1544.00		NIST Webbook
ripol	2153.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R409413&Units=SI
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

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