2H pyran-2-one,4-methyl-6-(2-methyl-1-propenyl)

Inchi: InChI=1S/C10H12O2/c1-7(2)4-9-5-8(3)6-10(11)12-9/h4-6H,1-3H3
InchiKey: BOYCIJXFRURCND-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(C)=Cc1cc(C)cc(=O)o1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	2.371		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R440147&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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