4-methyl-6-isopropyl-«alpha»-pyrone

Inchi: InChI=1S/C9H12O2/c1-6(2)8-4-7(3)5-9(10)11-8/h4-6H,1-3H3
InchiKey: YYWNAZJLTICGGQ-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: Cc1cc(C(C)C)oc(=O)c1
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.29		Crippen Method
logp	2.072		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
ripol	1862.00		NIST Webbook
ripol	1862.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R321605&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.