

(R)-9-((3,3-Dimethyl-2-oxiranyl)methoxy)-4-methoxy-7H-furo[3,2-g]chromen-7-one

Other names: (R)-9-((3,3-Dimethyloxiran-2-yl)methoxy)-4-methoxy-7H-furo[3,2-g]chromen-7-one
Inchi: InChI=1S/C17H16O6/c1-17(2)11(23-17)8-21-16-14-10(6-7-20-14)13(19-3)9-4-5-12(18)22
InchiKey: ORBITTMJKIGFNH-LLVKDONJSA-N
Formula: C17H16O6
SMILES: COc1c2ccoc2c(OCC2OC2(C)C)c2oc(=O)ccc12
Mol. weight [g/mol]: 316.31
CAS: 26091-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.09		Crippen Method
logp	3.104		Crippen Method
mcvol	216.370	ml/mol	McGowan Method
rinpol	2671.50		NIST Webbook
rinpol	2671.50		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C26091792&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

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