

(R,Z)-3-Hydroxy-3-methyl-1-((7-oxo-7H-furo[3,2-g]1,2-methylbut-2-enoate

InChI: InChI=1S/C21H22O7/c1-5-12(2)20(23)28-17(21(3,4)24)11-26-19-13-6-7-18(22)27-16(13)
InChIKey: WXULKGXQMWWMP-OMLDUKLJSA-N
Formula: C21H22O7
SMILES: CC=C(C)C(=O)OC(COc1c2ccoc2cc2oc(=O)ccc12)C(C)(C)O
Mol. weight [g/mol]: 386.40
CAS: 642-08-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.06		Crippen Method
logp	3.567		Crippen Method
mcvol	280.860	ml/mol	McGowan Method
rinpol	3048.80		NIST Webbook
rinpol	3048.80		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C642080&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

Latest version available from:
<https://www.chemeo.com/cid/84-661-5/R-Z-3-Hydroxy-3-methyl-1-7-oxo-7H-furo-3-2-g-chromen-4-yl-oxy-butan-2-yl-2>

Generated by Cheméo on 2025-12-05 17:39:37.706076472 +0000 UTC m=+4704575.236117136.

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