6,8-Dihydroxy-3-pentylisochromen-1-one (Olivetonide)

Inchi: InChI=1S/C14H16O4/c1-2-3-4-5-11-7-9-6-10(15)8-12(16)13(9)14(17)18-11/h6-8,15-16H,
InchiKey: FIMFRMRZGBUYMV-UHFFFAOYSA-N
Formula: C14H16O4
SMILES: CCCCCc1cc2cc(O)cc(O)c2c(=O)o1
Mol. weight [g/mol]: 248.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.59		Crippen Method
logp	2.937		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		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=R627933&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
rinpol: Non-polar retention indices

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