4-Hydroxycoumarin, pentafluoropropionate

Inchi: InChI=1S/C12H5F5O4/c13-11(14,12(15,16)17)10(19)21-8-5-9(18)20-7-4-2-1-3-6(7)8/h1-
InchiKey: UPQMSHVFIYAWIP-UHFFFAOYSA-N
Formula: C12H5F5O4
SMILES: O=C(Oc1cc(=O)oc2ccccc12)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 308.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.14		Crippen Method
logp	2.896		Crippen Method
mcvol	164.750	ml/mol	McGowan Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		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=U375582&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.