Chryseno[4,5-bcd]pyranone

Inchi: InChI=1S/C19H10O2/c20-19-15-10-12-4-1-2-6-13(12)14-9-8-11-5-3-7-16(21-19)17(11)18
InchiKey: XNMMIBUNQVKUQC-UHFFFAOYSA-N
Formula: C19H10O2
SMILES: O=c1oc2cccc3ccc4c5ccccc5cc1c4c32
Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.26		Crippen Method
logp	4.690		Crippen Method
mcvol	193.010	ml/mol	McGowan Method
rinpol	442.10		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R287822&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

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