3,10-Perylenequinone

Inchi: InChI=1S/C20H10O2/c21-17-9-7-13-14-8-10-18(22)16-6-2-4-12(20(14)16)11-3-1-5-15(17
InchiKey: FUTARTAINOHELR-UHFFFAOYSA-N
Formula: C20H10O2
SMILES: O=c1ccc2c3ccc(=O)c4cccc(c5cccc1c52)c43
Mol. weight [g/mol]: 282.29
CAS: 5796-93-0

Physical Properties

Property code	Value	Unit	Source
chs	-9029.00 ± 24.00	kJ/mol	NIST Webbook
log10ws	-6.36		Crippen Method
logp	3.895		Crippen Method
mcvol	202.800	ml/mol	McGowan Method

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=C5796930&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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