

Perylene-1,12-quinone

Inchi: InChI=1S/C20H10O2/c21-15-9-7-11-3-1-5-13-14-6-2-4-12-8-10-16(22)20(18(12)14)19(15)2
InchiKey: ODYASLOGAWBBOY-UHFFFAOYSA-N
Formula: C20H10O2
SMILES: O=c1ccc2cccc3c4cccc5ccc(=O)c(c1c23)c54
Mol. weight [g/mol]: 282.29
CAS: 5796-91-8

Physical Properties

Property code	Value	Unit	Source
chs	-9258.00 ± 52.00	kJ/mol	NIST Webbook
log10ws	-6.36		Crippen Method
logp	3.895		Crippen Method
mcvol	202.800	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5796918&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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