Dibenzo[drf,mno]chrysene, 2,3-dihydro

Other names: 2,3-dihydrodibenzo[def,mno]chrysene
Inchi: InChI=1S/C22H14/c1-3-13-7-9-18-12-16-6-2-4-14-8-10-17-11-15(5-1)19(13)21(18)22(17)
InchiKey: KDWIJRYPLQEXLS-UHFFFAOYSA-N
Formula: C22H14
SMILES: C1=c2cc3ccc4cccc5cc6ccc(c2c6c3c45)CC1
Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.24		Crippen Method
logp	5.183		Crippen Method
mcvol	212.680	ml/mol	McGowan Method
rinpol	503.91		NIST Webbook
rinpol	503.91		NIST Webbook
rinpol	503.91		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=R15507&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

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