

Cyclopenta[def]pyren-4-one

Inchi: InChI=1S/C17H10O/c18-15-16-7-1-3-11-5-6-12-4-2-8-17(15,10-9-16)14(12)13(11)16/h1-
InchiKey: IKRLZQBBTYFDNW-UHFFFAOYSA-N
Formula: C17H10O
SMILES: O=C1C23C=CC=c4ccc5c(c42)C1(C=CC=5)C=C3
Mol. weight [g/mol]: 230.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	1.015		Crippen Method
mcvol	167.560	ml/mol	McGowan Method
rinpol	2762.00		NIST Webbook
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Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R553129&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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<https://www.chemeo.com/cid/44-911-1/Cyclopenta-def-pyren-4-one.pdf>

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