

Indeno[1,2-a]phenalene

Inchi:	InChI=1S/C20H12/c1-2-9-17-14(5-1)11-16-12-15-8-3-6-13-7-4-10-18(19(13)15)20(16)17
InchiKey:	FKTWPJDLAUZQBF-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	C1=c2ccccc2=c2c1cc1cccc3cccc2c31
Mol. weight [g/mol]:	252.31
CAS:	198-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	4.141		Crippen Method
mvol	195.360	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=C198196&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
mvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/75-867-7/Indeno-1-2-a-phenalene.pdf>

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