

s-Indacene

Inchi:	InChI=1S/C12H8/c1-3-9-7-11-5-2-6-12(11)8-10(9)4-1/h1-8H
InchiKey:	WEMQMWWWCBYPOV-UHFFFAOYSA-N
Formula:	C12H8
SMILES:	<chem>C1=Cc2cc3c(cc2=C1)C=CC=3</chem>
Mol. weight [g/mol]:	152.19
CAS:	267-21-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.301		Crippen Method
mcvol	121.560	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C267210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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<https://www.chemeo.com/cid/79-472-1/s-Indacene.pdf>

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