

# Acenaphthylene[4,5-a]dibenzothiophene

<b>Inchi:</b>	InChI=1S/C22H12S/c1-2-7-18-16(5-1)22-19(23-18)11-10-15-12-14-9-8-13-4-3-6-17(20(1
<b>InchiKey:</b>	OWRNZBTXMZTPQY-UHFFFAOYSA-N
<b>Formula:</b>	C22H12S
<b>SMILES:</b>	C1=Cc2cc3ccc4sc5ccccc5c4c3c3ccc1c23
<b>Mol. weight [g/mol]:</b>	308.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.30		Crippen Method
logp	6.845		Crippen Method
mcvol	224.730	ml/mol	McGowan Method
rinpola	536.75		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R642432&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R642432&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpola:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/72-464-7/Acenaphthylene-4-5-a-dibenzothiophene.pdf>

Generated by Cheméo on 2024-04-26 14:07:42.075073165 +0000 UTC m=+16429710.995650478.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.