Anthra(1,2-b)thiophene

Other names:	Anthro[1,2-b]thiophene
Inchi:	InChI=1S/C16H10S/c1-2-4-13-10-15-14(9-12(13)3-1)6-5-11-7-8-17-16(11)15/h1-10H
InchiKey:	NMWGLCVKRMOELQ-UHFFFAOYSA-N
Formula:	C16H10S
SMILES:	c1ccc2cc3c(ccc4ccsc43)cc2c1
Mol. weight [g/mol]:	234.32
CAS:	227-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	5.208		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
rinpol	395.36		NIST Webbook
rinpol	395.34		NIST Webbook
rinpol	395.39		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C227861&Units=SI

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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