Benzo[7,8]anthro[2,1-b]thiophene, 5-methyl

Inchi:	InChI=1S/C21H14S/c1-13-8-21-18(6-7-22-21)20-12-17-10-15-5-3-2-4-14(15)9-16(17)11-
InchiKey:	RVCDUCKIZMLYJC-UHFFFAOYSA-N
Formula:	C21H14S
SMILES:	Cc1cc2sccc2c2cc3cc4ccccc4cc3cc12
Mol. weight [g/mol]:	298.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	6.669		Crippen Method
mcvol	225.800	ml/mol	McGowan Method
rinpol	511.30		NIST Webbook

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=R642581&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
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/77-527-2/Benzo-7-8-anthro-2-1-b-thiophene-5-methyl.pdf
Generated by Cheméo on 2024-10-12 08:22:41.549758341 +0000 UTC m=+3302224.186727590.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.