

Benzo[b]thiophene, 2-propyl-

Other names:	2-Propylbenzothiophene Benzothiophene, 2-propyl
Inchi:	InChI=1S/C11H12S/c1-2-5-10-8-9-6-3-4-7-11(9)12-10/h3-4,6-8H,2,5H2,1H3
InchiKey:	IBJARYHUXSJWRZ-UHFFFAOYSA-N
Formula:	C11H12S
SMILES:	CCc1cc2ccccc2s1
Mol. weight [g/mol]:	176.28
CAS:	16587-32-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.854		Crippen Method
mcvol	143.280	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16587329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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