

5-Ethylbenzo[b]thiophene

Other names:	Benzo[b]thiophene, 5-ethyl Benzothiophene, 5-ethyl
Inchi:	InChI=1S/C10H10S/c1-2-8-3-4-10-9(7-8)5-6-11-10/h3-7H,2H2,1H3
InchiKey:	XXKJPQUVYBHFBU-UHFFFAOYSA-N
Formula:	C10H10S
SMILES:	CCc1ccc2sccc2c1
Mol. weight [g/mol]:	162.25
CAS:	17514-96-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.464		Crippen Method
mcvol	129.190	ml/mol	McGowan Method
rinpol	236.14		NIST Webbook
rinpol	238.46		NIST Webbook
rinpol	236.14		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17514964&Units=SI
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

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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