

ethyl-benzothiophene

Inchi: InChI=1S/C10H10S/c1-2-9-7-8-5-3-4-6-10(8)11-9/h3-7H,2H2,1H3
InchiKey: JAABUGUCYZQMID-UHFFFAOYSA-N
Formula: C10H10S
SMILES: CCc1cc2ccccc2s1
Mol. weight [g/mol]: 162.25
CAS: 54385-63-6

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	235.00		NIST Webbook
rinpol	237.40		NIST Webbook
rinpol	235.00		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=C54385636&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

Latest version available from:

<https://www.chemeo.com/cid/79-607-1/ethyl-benzothiophene.pdf>

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