

Thiophene, 2-butyl-5-ethenyl

Other names: 2-Butyl-5-vinylthiophene
Inchi: InChI=1S/C10H14S/c1-3-5-6-10-8-7-9(4-2)11-10/h4,7-8H,2-3,5-6H2,1H3
InchiKey: JKFTXICJYSTDFO-UHFFFAOYSA-N
Formula: C10H14S
SMILES: C=Cc1ccc(CCCC)s1
Mol. weight [g/mol]: 166.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	3.734		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
rinpol	1256.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41762&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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<https://www.chemeo.com/cid/79-712-4/Thiophene-2-butyl-5-ethenyl.pdf>

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