

# Thiophene, 2-phenyl-

<b>Other names:</b>	2-Phenylthiophene
<b>Inchi:</b>	InChI=1S/C10H8S/c1-2-5-9(6-3-1)10-7-4-8-11-10/h1-8H
<b>InchiKey:</b>	PJRGDKFLFAYRBV-UHFFFAOYSA-N
<b>Formula:</b>	C10H8S
<b>SMILES:</b>	c1ccc(-c2cccs2)cc1
<b>Mol. weight [g/mol]:</b>	160.24
<b>CAS:</b>	825-55-8

## Physical Properties

Property code	Value	Unit	Source
ie	8.06	eV	NIST Webbook
log10ws	-3.83		Crippen Method
logp	3.415		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
rinpol	1376.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	2124.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C825558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C825558&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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