

# Thiophene, 3-ethyl-

<b>Other names:</b>	3-Ethylthiophene
<b>Inchi:</b>	InChI=1S/C6H8S/c1-2-6-3-4-7-5-6/h3-5H,2H2,1H3
<b>InchiKey:</b>	SLDBAXYJAIRQMX-UHFFFAOYSA-N
<b>Formula:</b>	C6H8S
<b>SMILES:</b>	CCc1ccsc1
<b>Mol. weight [g/mol]:</b>	112.19
<b>CAS:</b>	1795-01-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	2.310		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
ripol	866.00		NIST Webbook
ripol	872.00		NIST Webbook
ripol	850.00		NIST Webbook
ripol	872.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	862.00		NIST Webbook
ripol	862.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1211.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	40.70	kJ/mol	395.50	NIST Webbook

## Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43065e+01
Coeff. B	-3.37467e+03
Coeff. C	-5.99900e+01
Temperature range (K), min.	300.71
Temperature range (K), max.	435.16

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795013&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795013&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

## Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices

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