

# Thiophene, 3,4-dibromo-

Other names:	3,4-Dibromothiophene
Inchi:	InChI=1S/C4H2Br2S/c5-3-1-7-2-4(3)6/h1-2H
InchiKey:	VGKLVWTVUCUDISO-UHFFFAOYSA-N
Formula:	C4H2Br2S
SMILES:	BrC1cscC1Br
Mol. weight [g/mol]:	241.93
CAS:	3141-26-2

## Physical Properties

Property code	Value	Unit	Source
ie	8.94	eV	NIST Webbook
log10ws	-3.55		Crippen Method
logp	3.273		Crippen Method
mcvol	99.110	ml/mol	McGowan Method
rinpole	1267.00		NIST Webbook
rinpole	1267.00		NIST Webbook
tb	494.70	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	32.10	kJ/mol	353.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34269e+01
Coeff. B	-4.66212e+03
Coeff. C	3.46180e+01

Temperature range (K), min.	320.20
Temperature range (K), max.	539.86

## Sources

<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>
<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=C3141262&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3141262&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>

## Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<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>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/23-538-9/Thiophene-3-4-dibromo.pdf>

Generated by Cheméo on 2024-04-29 07:56:04.705240414 +0000 UTC m=+16666613.625817743.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.