

# Ethane, isothiocyanato-

<b>Other names:</b>	Ethyl isothiocyanate Ethyl mustard oil Isothiocyanatoethane Isothiocyanic acid, ethyl ester
<b>Inchi:</b>	InChI=1S/C3H5NS/c1-2-4-3-5/h2H2,1H3
<b>InchiKey:</b>	HBNYJWAFDZLWRS-UHFFFAOYSA-N
<b>Formula:</b>	C3H5NS
<b>SMILES:</b>	CCN=C=S
<b>Mol. weight [g/mol]:</b>	87.14
<b>CAS:</b>	542-85-8

## Physical Properties

Property code	Value	Unit	Source
hf	178.82	kJ/mol	Joback Method
hvap	39.80	kJ/mol	NIST Webbook
hvap	40.20	kJ/mol	NIST Webbook
ie	9.14 ± 0.03	eV	NIST Webbook
ie	9.10 ± 0.15	eV	NIST Webbook
ie	9.12 ± 0.05	eV	NIST Webbook
log10ws	-1.01		Crippen Method
logp	1.109		Crippen Method
mcvol	70.860	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	786.20		NIST Webbook
rinpol	786.20		NIST Webbook
tb	413.99	K	Joback Method
tc	637.78	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	106.30	J/mol×K	290.00	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.82008e+01
Coeff. B	-6.10748e+03
Coeff. C	4.50100e+01
Temperature range (K), min.	290.55
Temperature range (K), max.	428.83

## 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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C542858&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C542858&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>

## Legend

<b>cpl:</b>	Liquid phase heat capacity
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

Latest version available from:

<https://www.chemeo.com/cid/51-078-9/Ethane-isothiocyanato.pdf>

Generated by Cheméo on 2024-04-19 01:45:24.282610354 +0000 UTC m=+15780373.203187669.

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