

Thiazole

Other names:	1,3-thiazole
Inchi:	InChI=1S/C3H3NS/c1-2-5-3-4-1/h1-3H
InchiKey:	FZWLAAWBMGSTSO-UHFFFAOYSA-N
Formula:	C3H3NS
SMILES:	c1cscn1
Mol. weight [g/mol]:	85.13
CAS:	288-47-1

Physical Properties

Property code	Value	Unit	Source
affp	904.00	kJ/mol	NIST Webbook
basg	872.10	kJ/mol	NIST Webbook
cpl	122.10	J/mol×K	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
ie	9.50	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	1.143		Crippen Method
mcvol	60.000	ml/mol	McGowan Method
rinpol	711.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	694.00		NIST Webbook

rinpol	707.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	709.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1259.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1210.00		NIST Webbook
sl	169.95	J/mol×K	NIST Webbook
sl	169.95	J/mol×K	NIST Webbook

tb	391.39 ± 0.20	K	NIST Webbook
tb	390.70	K	NIST Webbook
tf	239.58 ± 0.05	K	NIST Webbook
tt	239.53 ± 0.02	K	NIST Webbook
tt	239.48 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	121.00	J/mol×K	298.15	NIST Webbook
cpl	121.00	J/mol×K	298.15	NIST Webbook
hfust	9.54	kJ/mol	239.53	NIST Webbook
hfust	9.59	kJ/mol	239.48	NIST Webbook
hfust	9.58	kJ/mol	239.40	NIST Webbook
hvapt	39.70	kJ/mol	363.00	NIST Webbook
hvapt	38.90	kJ/mol	363.50	NIST Webbook
sfust	40.04	J/mol×K	239.53	NIST Webbook
sfust	40.04	J/mol×K	239.48	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47286e+01
Coeff. B	-3.45024e+03
Coeff. C	-4.98900e+01
Temperature range (K), min.	288.81
Temperature range (K), max.	416.27

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C288471&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives: <https://www.doi.org/10.1016/j.tca.2005.11.024>
<https://www.cheric.org/files/research/kdb/mol/mol1463.mol>

Legend

affp:	Proton affinity
basg:	Gas basicity
cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/52-944-6/Thiazole.pdf>

Generated by Cheméo on 2025-12-05 08:20:45.141641524 +0000 UTC m=+4671042.671682179.

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