

Thiazole, tetrahydro-

Other names:	Thiazolidine Tetrahydrothiazole 1-Thia-3-azacyclopentane
Inchi:	InChI=1S/C3H7NS/c1-2-5-3-4-1/h4H,1-3H2
InchiKey:	OGYGFUAIOPWQD-UHFFFAOYSA-N
Formula:	C3H7NS
SMILES:	C1CSCN1
Mol. weight [g/mol]:	89.16
CAS:	504-78-9

Physical Properties

Property code	Value	Unit	Source
gf	146.21	kJ/mol	Joback Method
hf	58.64	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	35.41	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
logp	0.280		Crippen Method
mcvol	68.600	ml/mol	McGowan Method
pc	6161.14	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	903.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1460.00		NIST Webbook
tb	437.70	K	NIST Webbook
tc	614.68	K	Joback Method
tf	327.19	K	Joback Method
vc	0.229	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	107.14	J/mol×K	384.37	Joback Method
cpg	116.93	J/mol×K	422.76	Joback Method
cpg	126.15	J/mol×K	461.14	Joback Method
cpg	134.82	J/mol×K	499.53	Joback Method
cpg	142.96	J/mol×K	537.91	Joback Method
cpg	150.61	J/mol×K	576.30	Joback Method
cpg	157.77	J/mol×K	614.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.70	K	3.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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