

# 4(5H)-Thiazolone, 2-imino-

<b>Other names:</b>	2-Thiazolin-4-one, 2-amino- Pseudo-Thiohydantoin 2-Imino-4-thiazolidinone 2-Imino-4-thiazolidone 4-Thiazolidinone, 2-imino- USAF BE-4-5 USAF DM-1 2-Amino-thiazol-4-one 2-Amino-2-thiazolin-4-one 4(5H)-Thiazolone, 2-amino- NSC 2858 NSC 45956 2-imino-1,3-thiazol-4-one
<b>Inchi:</b>	InChI=1S/C3H4N2OS/c4-3-5-2(6)1-7-3/h1H2,(H2,4,5,6)
<b>InchiKey:</b>	HYMJHROUVPWYNQ-UHFFFAOYSA-N
<b>Formula:</b>	C3H4N2OS
<b>SMILES:</b>	<chem>N=C1NC(=O)CS1</chem>
<b>Mol. weight [g/mol]:</b>	116.14
<b>CAS:</b>	556-90-1

## Physical Properties

Property code	Value	Unit	Source
gf	201.01	kJ/mol	Joback Method
hf	87.87	kJ/mol	Joback Method
hvap	52.48	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	-0.216		Crippen Method
mcvol	75.850	ml/mol	McGowan Method
tb	539.13	K	Joback Method
tf	493.59	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	149.57	J/mol×K	539.13	Joback Method
cpg	41.06	J/mol×K	100.12	Joback Method
cpg	41.06	J/mol×K	100.12	Joback Method
cpg	41.06	J/mol×K	100.12	Joback Method
cpg	41.06	J/mol×K	100.12	Joback Method
cpg	41.06	J/mol×K	100.12	Joback Method
cpg	41.06	J/mol×K	100.12	Joback Method
cps	106.00	J/mol×K	277.80	NIST Webbook

## Sources

<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=C556901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C556901&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<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>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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