

# 2-Propenethioamide, 2-cyano-3-phenyl-, (E)-

<b>Inchi:</b>	InChI=1S/C10H8N2S/c11-7-9(10(12)13)6-8-4-2-1-3-5-8/h1-6H,(H2,12,13)/b9-6+
<b>InchiKey:</b>	DFVRLZLNOKWNEH-RMKNXTFCSA-N
<b>Formula:</b>	C10H8N2S
<b>SMILES:</b>	N#CC(=Cc1ccccc1)C(=N)S
<b>Mol. weight [g/mol]:</b>	188.25
<b>CAS:</b>	68029-52-7

## Physical Properties

Property code	Value	Unit	Source
gf	583.57	kJ/mol	Joback Method
hf	495.92	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	2.501		Crippen Method
mcvol	147.110	ml/mol	McGowan Method
tb	708.20	K	Joback Method
tf	380.07	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.63	J/molxK	708.20	Joback Method
cpg	45.79	J/molxK	100.12	Joback Method
cpg	45.79	J/molxK	100.12	Joback Method
cpg	45.79	J/molxK	100.12	Joback Method
cpg	45.79	J/molxK	100.12	Joback Method
cpg	45.79	J/molxK	100.12	Joback Method
cpg	45.79	J/molxK	100.12	Joback Method

## Sources

<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=C68029527&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C68029527&amp;Units=SI</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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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