

# 2-pyridinecarbothioamide

<b>Other names:</b>	pyridine-2-carbothioamide thiopicolinamide
<b>Inchi:</b>	InChI=1S/C6H6N2S/c7-6(9)5-3-1-2-4-8-5/h1-4H,(H2,7,9)
<b>InchiKey:</b>	HYKQYVSNFPWGKQ-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2S
<b>SMILES:</b>	NC(=S)c1ccccn1
<b>Mol. weight [g/mol]:</b>	138.20

## Physical Properties

Property code	Value	Unit	Source
hfus	25.30	kJ/mol	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
log10ws	-2.01		Crippen Method
logp	0.716		Crippen Method
mcvol	103.650	ml/mol	McGowan Method
tf	407.00	K	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	7.99e-04	kPa	333.65	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method

psub	9.00e-04	kPa	335.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	1.08e-03	kPa	337.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	1.22e-03	kPa	339.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	1.50e-03	kPa	341.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	1.86e-03	kPa	343.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	2.19e-03	kPa	345.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	2.66e-03	kPa	347.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method

psub	3.05e-03	kPa	349.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	3.74e-03	kPa	351.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	4.21e-03	kPa	353.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method
psub	5.19e-03	kPa	355.15	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method

## Sources

<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>
<b>Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method:</b>	<a href="https://www.doi.org/10.1016/j.tca.2015.10.009">https://www.doi.org/10.1016/j.tca.2015.10.009</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>hfus:</b>	Enthalpy of fusion 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

**psub:** Sublimation pressure  
**tf:** Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/107-863-5/2-pyridinecarbothioamide.pdf>

Generated by Cheméo on 2024-04-29 11:03:38.788969885 +0000 UTC m=+16677867.709547208.

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