

2-pyridinecarbothioamide

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method:	https://www.doi.org/10.1016/j.tca.2015.10.009
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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

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