Protionamide

Other names:	4-Pyridinecarbothioamide, 2-propyl- Isonicotinamide, 2-propylthio- Ektebin Peteha 2-Propylisonicotinylthioamide 2-Propyl-4-pyridinecarbothioamide 2-Propyl-4-thiocarbamoylpyridine 2-Propyl-thioisonicotinamide Prothionamide Protion Protionamid Protionizina 9778 R.P. Tebeform 1321 TH Trevintix Tuberex RP-9778 TH-1321
Inchi:	InChI=1S/C9H12N2S/c1-2-3-8-6-7(9(10)12)4-5-11-8/h4-6H,2-3H2,1H3,(H2,10,12)
InchiKey:	VRDIULHPQTYCLN-UHFFFAOYSA-N
Formula:	C9H12N2S
SMILES:	CCCc1cc(C(=N)S)ccn1
Mol. weight [g/mol]:	180.27
CAS:	14222-60-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	2.289		Crippen Method
mcvol	145.920	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.21	kJ/mol	414.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14222607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume