

Ethionamide

Other names: 1314 TH
1314 TN
2-Ethyl-4-thioamidylpyridine
2-Ethyl-4-thiocarbamoylpyridine
2-Ethylisonicotinic acid thioamide
2-Ethylisonicotinothiamide
2-Ethylisonicotinothioamide
2-Ethylisonicotinthioamide
2-Ethylisothionicotinamide
2-ethyl-4-pyridinecarbothioamide
2-ethylpyridine-4-carbothioamide
2-ethylthioisonicotinamide
4-Pyridinecarbothioamide, 2-ethyl-
Aetina
Aetiva
Amidazin
Amidazine
Atina
Bayer 5312
ETP
Ethimide
Ethina
Ethinamide
Ethionamid prothionamid
Ethionamide
Ethylisothiamide
Ethyonomide
Etimid
Etiocidan
Etionamid
Etioniamid
Etionid
Etionizin
Etionizina
Etionizine
F.I. 58-30
Fatoliamid
Iridocin
Iridocin Bayer
Iridozin

Isonicotinamide, 2-ethyl, thio-
Isothin
Isotiamida
Itiocide
NCI-C01694
Nicotion
Nisotin
Nizotin
Rigenicid
Sertinon
Teberus
Th 1314
Thianid
Thianide
Thioamide
Thiodine
Thiomid
Thioniden
Tianid
Tiomid
Trecator
Trecator-SC
Trekator
Trescatyl
Trescazole
Tubenamide
Tubermin
Tuberoid
Tuberoson
«alpha»-Ethylisonicotinic acid thioamide
«alpha»-Ethylisonicotinoylthioamide
«alpha»-Ethylisothionicotinamide
«alpha»-Ethylthioisonicotinamide

Inchi: InChI=1S/C8H10N2S/c1-2-7-5-6(8(9)11)3-4-10-7/h3-5H,2H2,1H3,(H2,9,11)

InchiKey: AEOCXXJPGCBFJA-UHFFFAOYSA-N

Formula: C8H10N2S

SMILES: CCc1cc(C(N)=S)ccn1

Mol. weight [g/mol]: 166.24

CAS: 536-33-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.278		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
rinpol	1756.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tf	435.90	K	Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C536334&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Studying the sublimation thermodynamics of ethionamide and pyridine carbothioamide isomers by transpiration method in buffer solutions, octanol and hexane at several temperatures:

<https://www.doi.org/10.1016/j.tca.2015.10.009>

<https://www.doi.org/10.1016/j.tca.2016.07.020>

<http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mccvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/31-632-5/Ethionamide.pdf>

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