

# 5-Pyrimidinecarboxylic acid, 4-amino-2-(ethylthio)-

Inchi:	InChI=1S/C7H9N3O2S/c1-2-13-7-9-3-4(6(11)12)5(8)10-7/h3H,2H2,1H3,(H,11,12)(H2,8,9)
InchiKey:	TYAKXNHFMATCHA-UHFFFAOYSA-N
Formula:	C7H9N3O2S
SMILES:	CCSc1ncc(C(=O)O)c(N)n1
Mol. weight [g/mol]:	199.23
CAS:	89853-87-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	0.869		Crippen Method
mcvol	139.460	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C89853872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89853872&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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