

6-Amino-2-(ethylthio)-4-pyrimidinol

Other names:	6-amino-2-(ethylthio)-1H-pyrimidin-4-one
Inchi:	InChI=1S/C6H9N3OS/c1-2-11-6-8-4(7)3-5(10)9-6/h3H,2H2,1H3,(H3,7,8,9,10)
InchiKey:	OYIIQANZEPQOV-UHFFFAOYSA-N
Formula:	C6H9N3OS
SMILES:	CCSc1nc(N)cc(O)n1
Mol. weight [g/mol]:	171.22
CAS:	37660-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	0.876		Crippen Method
mcvol	123.800	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37660223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/19-795-9/6-Amino-2-ethylthio-4-pyrimidinol.pdf>

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