

2,4-Diamino-6-ethoxypyrimidine

Inchi:	InChI=1S/C6H10N4O/c1-2-11-5-3-4(7)9-6(8)10-5/h3H,2H2,1H3,(H4,7,8,9,10)
InchiKey:	MMTAQMVMXGXVICH-UHFFFAOYSA-N
Formula:	C6H10N4O
SMILES:	CCOc1cc(N)[nH]c(=N)n1
Mol. weight [g/mol]:	154.17
CAS:	116436-03-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	-0.612		Crippen Method
mcvol	117.430	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436034&Units=SI

Legend

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

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