

Pyrimido[5,4-e]-as-triazine, 5-(ethylamino)-

Inchi:	InChI=1S/C7H8N6/c1-2-8-6-5-7(11-3-10-6)13-12-4-9-5/h3-4H,2H2,1H3,(H,8,10,11,13)
InchiKey:	UJMZFVINWRRUAF-UHFFFAOYSA-N
Formula:	C7H8N6
SMILES:	CCNc1ncnc2nncnc12
Mol. weight [g/mol]:	176.18
CAS:	19359-60-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	0.247		Crippen Method
mcvol	126.150	ml/mol	McGowan Method

Sources

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=C19359605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/38-429-4/Pyrimido-5-4-e-as-triazine-5-ethylamino.pdf>

Generated by Cheméo on 2024-04-20 12:08:45.826630985 +0000 UTC m=+15904174.747208308.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.