

As-triazine-5-carboxamide, 6-amino-n-ethyl-

Inchi:	InChI=1S/C6H10N6/c1-2-9-5(7)4-6(8)12-11-3-10-4/h3H,2H2,1H3,(H2,7,9)(H2,8,12)
InchiKey:	YRBYHGOQFSCMA-UHFFFAOYSA-N
Formula:	C6H10N6
SMILES:	CCN=C(N)c1ncnc1N
Mol. weight [g/mol]:	166.18
CAS:	19359-62-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	-0.821		Crippen Method
mcvol	127.220	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=C19359627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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