

Pyrimidine, 4,6-dichloro-2-ethyl-

Inchi:	InChI=1S/C6H6Cl2N2/c1-2-6-9-4(7)3-5(8)10-6/h3H,2H2,1H3
InchiKey:	WASNBYSRKJXRFGU-UHFFFAOYSA-N
Formula:	C6H6Cl2N2
SMILES:	CCc1nc(Cl)cc(Cl)n1
Mol. weight [g/mol]:	177.03
CAS:	1195-34-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.346		Crippen Method
mcvol	116.080	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=C1195342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/125-094-9/Pyrimidine-4-6-dichloro-2-ethyl.pdf>

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