

1-(2-Cyanoethyl)-2-ethyl-4-methylimidazole

Other names:	1H-Imidazole-1-propanenitrile, 2-ethyl-4-methyl-1-Cyanoethyl-2-ethyl-4-methylimidazole 2-ethyl-4-methyl-1H-imidazole-1-propiononitrile
Inchi:	InChI=1S/C9H13N3/c1-3-9-11-8(2)7-12(9)6-4-5-10/h7H,3-4,6H2,1-2H3
InchiKey:	UDDPPKZYZTEGS-UHFFFAOYSA-N
Formula:	C9H13N3
SMILES:	CCc1nc(C)cn1CCC#N
Mol. weight [g/mol]:	163.22
CAS:	23996-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.668		Crippen Method
mcvol	139.550	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23996250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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