

1,4-Piperazinediacetonitrile, alpha, alpha', 2,5-tetramethyl-, trans-

Inchi:	InChI=1S/C12H20N4/c1-9(5-13)15-7-12(4)16(8-11(15)3)10(2)6-14/h9-12H,7-8H2,1-4H3
InchiKey:	RLWOJDBOCLGZSD-UHFFFAOYSA-N
Formula:	C12H20N4
SMILES:	CC(C#N)N1CC(C)N(C(C)C#N)CC1C
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	1.205		Crippen Method
mcvol	191.800	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6005698&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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