

1,4-Piperazinediacetonitrile, alpha, alpha', 2-trimethyl-

Inchi:	InChI=1S/C11H18N4/c1-9(6-12)14-4-5-15(10(2)7-13)11(3)8-14/h9-11H,4-5,8H2,1-3H3
InchiKey:	ACWGKNMPTHRMGE-UHFFFAOYSA-N
Formula:	C11H18N4
SMILES:	CC(C#N)N1CCN(C(C)C#N)C(C)C1
Mol. weight [g/mol]:	206.29
CAS:	92059-12-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	0.817		Crippen Method
mcvol	177.710	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=C92059126&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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