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