

# 1,4-Piperazinedipropionic acid, dimethyl ester

<b>Other names:</b>	dimethyl piperazine-1,4-dipropionate
<b>Inchi:</b>	InChI=1S/C12H22N2O4/c1-17-11(15)3-5-13-7-9-14(10-8-13)6-4-12(16)18-2/h3-10H2,1-2
<b>InchiKey:</b>	ZNYIVYFFZCEWDY-UHFFFAOYSA-N
<b>Formula:</b>	C12H22N2O4
<b>SMILES:</b>	COC(=O)CCN1CCN(CCC(=O)OC)CC1
<b>Mol. weight [g/mol]:</b>	258.31
<b>CAS:</b>	4038-90-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.39		Crippen Method
logp	-0.270		Crippen Method
mcvol	203.920	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4038908&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4038908&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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