

1,4-Bis-(2-hydroxypropyl)-2-methylpiperazine

Other names:	3,3'-(2-methylpiperazine-1,4-diyl)dipropan-2-ol
Inchi:	InChI=1S/C11H24N2O2/c1-9-6-12(7-10(2)14)4-5-13(9)8-11(3)15/h9-11,14-15H,4-8H2,1-
InchiKey:	GPXSTLAIBOEFST-UHFFFAOYSA-N
Formula:	C11H24N2O2
SMILES:	CC(O)CN1CCN(CC(C)O)C(C)C1
Mol. weight [g/mol]:	216.32
CAS:	94-72-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	-0.246		Crippen Method
mcvol	186.690	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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