

2,5-Dimethyl-1,4-dipropionitrile piperazine

Inchi:	InChI=1S/C12H20N4/c1-11-9-16(8-4-6-14)12(2)10-15(11)7-3-5-13/h11-12H,3-4,7-10H2,
InchiKey:	WBVQHDFSBWONKW-UHFFFAOYSA-N
Formula:	C12H20N4
SMILES:	CC1CN(CCC#N)C(C)CN1CCC#N
Mol. weight [g/mol]:	220.31
CAS:	4236-65-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.84		Crippen Method
logp	1.208		Crippen Method
mcvol	191.800	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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=C4236651&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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