

# Butyronitrile, 4-diisopropylamino-2-phenyl-2-(2-pyridyl)-

Other names:	«alpha»-[2-[bis(isopropyl)amino]ethyl]-«alpha»-phenylpyridine-2-acetonitrile
Inchi:	InChI=1S/C21H27N3/c1-17(2)24(18(3)4)15-13-21(16-22,19-10-6-5-7-11-19)20-12-8-9-14
InchiKey:	SSDIPWVVFVRNKB-UHFFFAOYSA-N
Formula:	C21H27N3
SMILES:	CC(C)N(CCC(C#N)(c1ccccc1)c1cccn1)C(C)C
Mol. weight [g/mol]:	321.46
CAS:	5005-46-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	4.400		Crippen Method
mcvol	280.570	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5005469&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5005469&amp;Units=SI</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/96-260-7/Butyronitrile-4-diisopropylamino-2-phenyl-2-2-pyridyl.pdf>

Generated by Cheméo on 2024-04-28 21:45:22.13285288 +0000 UTC m=+16629971.053430196.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.