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: SSDIPWVFVFRNKB-UHFFFAOYSA-N
Formula: C21H27N3
SMILES: CC(C)N(CCC(C#N)(c1ccccc1)c1ccccn1)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: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5005469&Units=SI

Legend

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