Benzylmorphine

Other names:	3-O-benzylmorphine 7,8-Didehydro-4,5-epoxy-17-methyl-3-(phenylmethoxy)morphinan-6-ol Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-17-methyl-3-(phenylmethoxy)-, (5«alpha» 6«alpha»)- Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-17-methyl-3-(phenylmethoxy)-, (5Â«alphaÂ» 6Â«alphaÂ»)- Morphinan-6-«alpha»-ol, 3-(benzyloxy)-7,8-didehydro-4,5-«alpha»-epoxy-17-methyl- Morphinan-6-Â«alphaÂ»-ol, 3-(benzyloxy)-7,8-didehydro-4,5-Â«alphaÂ»-epoxy-17-methyl- Morphinan-6«alpha»-ol, 3-(benzyloxy)-7,8-didehydro-4,5«alpha»-epxoy-17-methyl- Morphinan-6Â«alphaÂ»-ol, 3-(benzyloxy)-7,8-didehydro-4,5Â«alphaÂ»-epxoy-17-methyl- Morphine, benzyl- O3-Benzylmorphine
Inchi:	InChI=1S/C24H25NO3/c1-25-12-11-24-17-8-9-19(26)23(24)28-22-20(27-14-15-5-3-2-4-6
InchiKey:	RDJGWRFTDZZXSM-UHFFFAOYSA-N
Formula:	C24H25NO3
SMILES:	CN1CCC23c4c5ccc(OCc6ccccc6)c4OC2C(O)C=CC3C1C5
Mol. weight [g/mol]:	375.46
CAS:	14297-87-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Aqueous Solubility Prediction Method
logp	3.072		Crippen Method
mcvol	281.350	ml/mol	McGowan Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14297871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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