

Naltrexone

Other names:

Morphinan-6-one, 17-(cyclopropylmethyl)-4,5-epoxy-3,14-dihydroxy-, (5«alpha»)-
Morphinan-6-one, 17-(cyclopropylmethyl)-4,5-«alpha»-epoxy-3,14-dihydroxy-
17-(Cyclopropylmethyl)-4,5-epoxy-3,14-dihydroxymorphinan-6-one
N-Cyclopropylmethyl-14-hydroxydihydromorphinone
N-Cyclopropylmethylnoroxymorphone
EN 1639
EN 1939
UM-792
17-(Cyclopropylmethyl)-4,5«alpha»-epoxy-3,14-dihydroxymorphinan-6-one
ReVia
Vivitrex
Vivitrol

Inchi: InChI=1S/C20H23NO4/c22-13-4-3-12-9-15-20(24)6-5-14(23)18-19(20,16(12)17(13)25-18**InchiKey:** DQCKKXVULJGBQN-UHFFFAOYSA-N**Formula:** C20H23NO4**SMILES:** O=C1CCC2(O)C3Cc4ccc(O)c5c4C2(CCN3CC2CC2)C1O5**Mol. weight [g/mol]:** 341.40**CAS:** 16590-41-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	1.525		Crippen Method
mcpvol	243.760	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.80	kJ/mol	448.90	NIST Webbook
hfust	15.64	kJ/mol	448.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16590413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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