BUPRENORPHINE

Other names:	17-(Cyclopropylmethyl)-«alpha»-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy- 6,14-Ethenomorphinan-7-methanol, 17-(cyclopropylmethyl)-«alpha»-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-3-hydroxy-6 (5-«alpha»,7-«alpha»-(S))- RX 6029M Temgesic [5«alpha»,7«alpha»(S)]-17-(Cyclopropylmethyl)-«alpha»-(1,1-dimethylethyl)-4,5-epoxy-18
Inchi:	InChI=1S/C29H41NO4/c1-25(2,3)26(4,32)20-15-27-10-11-29(20,33-5)24-28(27)12-13-30
InchiKey:	RMRJXGBAOAMLHD-UHFFFAOYSA-N
Formula:	C29H41NO4
SMILES:	COC12CCC3(CC1C(C)(O)C(C)(C)C)C1Cc4ccc(O)c5c4C3(CCN1CC1CC1)C2O5
Mol. weight [g/mol]:	467.65

Physical Properties

Property code	Value	Unit	Source
logp	4.414		Crippen Method
mcvol	364.010	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.80	kJ/mol	491.30	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52485797&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume