DIPROPANOYLMORPHINE

Other names:	Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl- (5«alpha»,6«alpha»)-, dipropanoate Morphine dipropanoate Morphine, propionate Morphine, propionic ester 3,6-O-Dipropionylmorphine (5«alpha»,6«alpha»)-7,8-didehydro-4,5-epoxy-17-methylmorphinan-3,6-diyl dipropionate
Inchi:	InChI=1S/C23H27NO5/c1-4-18(25)27-16-8-6-13-12-15-14-7-9-17(28-19(26)5-2)22-23(14
InchiKey:	MTPLCRHXXMCRGG-UHFFFAOYSA-N
Formula:	C23H27NO5
SMILES:	CCC(=O)Oc1ccc2c3c1OC1C(OC(=O)CC)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	397.47

Physical Properties

Property code	Value	Unit	Source
ie	7.94	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	2.769		Crippen Method
mcvol	294.160	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tf	390.12	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C10589794&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point