ethylmorphine, propionic ester

Inchi: InChI=1S/C22H27NO4/c1-4-18(24)26-17-9-7-14-15-12-13-6-8-16(25-5-2)20-19(13)22(14
InchiKey: GICGOCRNVALHOZ-BIOFEAMMSA-N
Formula: C22H27NO4
SMILES: CCOc1ccc2c3c1OC1C(OC(=O)CC)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Crippen Method
logp	2.852		Crippen Method
mcvol	278.500	ml/mol	McGowan Method
rinpol	2700.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R407511&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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