

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
rinpola	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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/42-426-2/ethylmorphine-propionic-ester.pdf>

Generated by Cheméo on 2024-04-25 08:02:12.995538141 +0000 UTC m=+16321381.916115463.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.