3«beta»-Feruloyloxytropane

Inchi: InChI=1S/C18H23NO4/c1-19-13-5-6-14(19)11-15(10-13)23-18(21)8-4-12-3-7-16(20)17(9
InchiKey: RSPBFOSKTPFBGJ-RRJKNOHSSA-N
Formula: C18H23NO4
SMILES: COc1cc(C=CC(=O)OC2CC3CCC(C2)N3C)ccc1O
Mol. weight [g/mol]: 317.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.582		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
rinpol	2738.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R509647&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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