Desethylretusamine

Inchi: InChI=1S/C17H21NO7/c1-9-12-14(20)24-11-5-7-18(3)6-4-10(13(11)19)8-23-16(22)17(9,2
InchiKey: LMDYPJAYQRYLOD-NHNHHMODSA-N
Formula: C17H21NO7
SMILES: CC1C2C(=O)OC3CCN(C)CC=C(COC(=O)C1(C)OC2=O)C3=O
Mol. weight [g/mol]: 351.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.65		Crippen Method
logp	-0.146		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R590282&Units=SI

Legend

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

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