8E,10E-Dodecadienyl acetate + MTAD adduct

Inchi: InChI=1S/C17H27N3O4/c1-13-10-11-15(20-17(23)18(3)16(22)19(13)20)9-7-5-4-6-8-12-2
InchiKey: PMZMIFPAYRRFCE-UHFFFAOYSA-N
Formula: C17H27N3O4
SMILES: CC(=O)OCCCCCCCCC1C=CC(C)n2c(=O)n(C)c(=O)n21
Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	1.924		Crippen Method
mcvol	264.890	ml/mol	McGowan Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R219453&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

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