Trazodone -M (N-desalkyl-HO-) isomer-1 2AC

Inchi: InChI=1S/C14H17ClN2O3/c1-10(18)16-5-7-17(8-6-16)12-3-4-14(13(15)9-12)20-11(2)19/
InchiKey: VFJMBFXTQVURJB-UHFFFAOYSA-N
Formula: C14H17ClN2O3
SMILES: CC(=O)Oc1ccc(N2CCN(C(C)=O)CC2)cc1Cl
Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
ie	7.89	eV	Cheméo Relay (1.0)
logp	1.934		Crippen Method
mcvol	214.710	ml/mol	McGowan Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	630.91	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R331132&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature