Tolpropamine M (bis-nor, OH, -H2O), acetylated

Inchi: InChI=1S/C18H19NO/c1-14-8-10-17(11-9-14)18(12-13-19-15(2)20)16-6-4-3-5-7-16/h3-12

InchiKey: SLYPVQWEMDMFHL-LDADJPATSA-N

Formula: C18H19NO

SMILES: CC(O)=NCC=C(c1ccccc1)c1ccc(C)cc1

Mol. weight [g/mol]: 265.35

Physical Properties

Property code	Value	Unit	Source
hf	74.37	kJ/mol	Joback Method
hvap	80.99	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.403		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	2560.00		NIST Webbook
tb	842.36	K	Joback Method
tc	1075.27	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120779&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature