Tolpropamine M (bis-nor), acetylated

Inchi: InChI=1S/C18H21NO/c1-14-8-10-17(11-9-14)18(12-13-19-15(2)20)16-6-4-3-5-7-16/h3-1
InchiKey: OETWYHPMGLYEQG-UHFFFAOYSA-N
Formula: C18H21NO
SMILES: CC(O)=NCCC(c1ccccc1)c1ccc(C)cc1
Mol. weight [g/mol]: 267.37

Physical Properties

Property code	Value	Unit	Source
hf	-38.34	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.493		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	837.88	K	Joback Method
tc	1064.40	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=R120764&Units=SI

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