Tolpropamine M (norhydroxyalkyl, -H2O), acetylated

Inchi: InChI=1S/C19H21NO/c1-15-9-11-18(12-10-15)19(13-14-20(3)16(2)21)17-7-5-4-6-8-17/h4

InchiKey: OTYNUTAHQCLIBS-UYRXBGFRSA-N

Formula: C19H21NO

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

Mol. weight [g/mol]: 279.38

Physical Properties

Property code	Value	Unit	Source
gf	377.82	kJ/mol	Joback Method
hf	88.48	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.905		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2585.00		NIST Webbook
tb	762.81	K	Joback Method
tc	995.66	K	Joback Method
tf	432.61	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.07	J/mol×K	762.81	Joback Method
cpg	686.07	J/mol×K	801.62	Joback Method
cpg	701.81	J/mol×K	840.43	Joback Method
cpg	716.40	J/mol×K	879.23	Joback Method
cpg	729.95	J/mol×K	918.04	Joback Method
cpg	742.58	J/mol×K	956.85	Joback Method
cpg	754.39	J/mol×K	995.66	Joback Method

Sources

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=R314622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume