Tolpropamine M (nor), acetylated

Inchi: InChI=1S/C19H23NO/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: ZDFPDKOJGBPWSV-UHFFFAOYSA-N
Formula: C19H23NO
SMILES: CC(=O)N(C)CCC(c1ccccc1)c1ccc(C)cc1
Mol. weight [g/mol]: 281.39

Physical Properties

Property code	Value	Unit	Source
gf	303.71	kJ/mol	Joback Method
hf	-24.23	kJ/mol	Joback Method
hfus	33.76	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.995		Crippen Method
mcvol	242.600	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	758.33	K	Joback Method
tc	983.77	K	Joback Method
tf	436.65	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.59	J/mol×K	758.33	Joback Method
cpg	712.16	J/mol×K	795.90	Joback Method
cpg	728.42	J/mol×K	833.48	Joback Method
cpg	743.46	J/mol×K	871.05	Joback Method
cpg	757.38	J/mol×K	908.62	Joback Method
cpg	770.26	J/mol×K	946.20	Joback Method
cpg	782.18	J/mol×K	983.77	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=R120784&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