Tolpropamine M (OH), acetylated

Inchi: InChI=1S/C20H25NO2/c1-16-10-12-19(13-11-16)20(23-17(2)22,14-15-21(3)4)18-8-6-5-7
InchiKey: WRGYCGKOOWZHJR-UHFFFAOYSA-N
Formula: C20H25NO2
SMILES: CC(=O)OC(CCN(C)C)(c1ccccc1)c1ccc(C)cc1
Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	212.41	kJ/mol	Joback Method
hf	-180.56	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	75.23	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.753		Crippen Method
mcvol	262.560	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	2250.00		NIST Webbook
tb	800.84	K	Joback Method
tc	1027.40	K	Joback Method
tf	487.57	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.99	J/mol×K	800.84	Joback Method
cpg	798.20	J/mol×K	838.60	Joback Method
cpg	814.10	J/mol×K	876.36	Joback Method
cpg	828.77	J/mol×K	914.12	Joback Method
cpg	842.30	J/mol×K	951.88	Joback Method
cpg	854.81	J/mol×K	989.64	Joback Method
cpg	866.38	J/mol×K	1027.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120799&Units=SI
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

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