Tolpropamine M (OH-aryl), acetylated

Inchi: InChI=1S/C20H25NO2/c1-15-5-7-17(8-6-15)20(13-14-21(3)4)18-9-11-19(12-10-18)23-16
InchiKey: UFRWHKUADVBYMC-UHFFFAOYSA-N
Formula: C20H25NO2
SMILES: CC(=O)Oc1ccc(C(CCN(C)C)c2ccc(C)cc2)cc1
Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	197.50	kJ/mol	Joback Method
hf	-188.56	kJ/mol	Joback Method
hfus	37.14	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.004		Crippen Method
mcvol	262.560	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	808.61	K	Joback Method
tc	1029.64	K	Joback Method
tf	482.67	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.30	J/mol×K	808.61	Joback Method
cpg	796.23	J/mol×K	845.45	Joback Method
cpg	811.89	J/mol×K	882.29	Joback Method
cpg	826.34	J/mol×K	919.12	Joback Method
cpg	839.63	J/mol×K	955.96	Joback Method
cpg	851.84	J/mol×K	992.80	Joback Method
cpg	863.01	J/mol×K	1029.64	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=R120808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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