Metoprolol - H2O, acetylated

Inchi: InChI=1S/C17H25NO3/c1-14(2)18(15(3)19)11-5-12-21-17-8-6-16(7-9-17)10-13-20-4/h5-9
InchiKey: ANCVPHJOUAZRNS-VZUCSPMQSA-N
Formula: C17H25NO3
SMILES: COCCc1ccc(OCC=CN(C(C)=O)C(C)C)cc1
Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	44.68	kJ/mol	Joback Method
hf	-366.70	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.025		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	734.89	K	Joback Method
tc	935.72	K	Joback Method
tf	427.07	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.65	J/mol×K	734.89	Joback Method
cpg	718.52	J/mol×K	768.36	Joback Method
cpg	734.35	J/mol×K	801.83	Joback Method
cpg	749.18	J/mol×K	835.31	Joback Method
cpg	763.05	J/mol×K	868.78	Joback Method
cpg	775.99	J/mol×K	902.25	Joback Method
cpg	788.04	J/mol×K	935.72	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=R582751&Units=SI

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