Propranolol - H2O, acetylated

Inchi: InChI=1S/C18H21NO2/c1-14(2)19(15(3)20)12-7-13-21-18-11-6-9-16-8-4-5-10-17(16)18/h
InchiKey: XQYBCWDGDFEQAV-GHXNOFRVSA-N
Formula: C18H21NO2
SMILES: CC(=O)N(C=CCOc1cccc2ccccc12)C(C)C
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	264.75	kJ/mol	Joback Method
hf	-64.05	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	71.01	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.989		Crippen Method
mcvol	234.380	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	754.33	K	Joback Method
tc	974.69	K	Joback Method
tf	448.81	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.78	J/mol×K	754.33	Joback Method
cpg	677.82	J/mol×K	791.06	Joback Method
cpg	692.77	J/mol×K	827.78	Joback Method
cpg	706.73	J/mol×K	864.51	Joback Method
cpg	719.79	J/mol×K	901.24	Joback Method
cpg	732.03	J/mol×K	937.97	Joback Method
cpg	743.55	J/mol×K	974.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582999&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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