Bupranolol, acetylated

Inchi: InChI=1S/C18H26ClNO4/c1-12-7-8-16(19)17(9-12)23-11-15(24-14(3)22)10-20(13(2)21)1
InchiKey: WNAOOIQGLFGOIG-UHFFFAOYSA-N
Formula: C18H26ClNO4
SMILES: CC(=O)OC(COc1cc(C)ccc1Cl)CN(C(C)=O)C(C)(C)C
Mol. weight [g/mol]: 355.86

Physical Properties

Property code	Value	Unit	Source
gf	-174.76	kJ/mol	Joback Method
hf	-653.10	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	82.32	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.606		Crippen Method
mcvol	277.820	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2370.00		NIST Webbook
tb	846.66	K	Joback Method
tc	1059.32	K	Joback Method
tf	538.21	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.77	J/mol×K	846.66	Joback Method
cpg	845.54	J/mol×K	882.10	Joback Method
cpg	859.17	J/mol×K	917.55	Joback Method
cpg	871.70	J/mol×K	952.99	Joback Method
cpg	883.18	J/mol×K	988.43	Joback Method
cpg	893.65	J/mol×K	1023.88	Joback Method
cpg	903.16	J/mol×K	1059.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582553&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