Atenolol diacetate

Other names: Atenolol, acetylated
Inchi: InChI=1S/C18H26N2O5/c1-12(2)20(13(3)21)10-17(25-14(4)22)11-24-16-7-5-15(6-8-16)9
InchiKey: QRLMZEGBCRPZKY-UHFFFAOYSA-N
Formula: C18H26N2O5
SMILES: CC(=O)OC(COc1ccc(CC(N)=O)cc1)CN(C(C)=O)C(C)C
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-220.95	kJ/mol	Joback Method
hf	-701.21	kJ/mol	Joback Method
hfus	44.37	kJ/mol	Joback Method
hvap	95.57	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.282		Crippen Method
mcvol	277.130	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	933.44	K	Joback Method
tc	1153.33	K	Joback Method
tf	611.54	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.64	J/mol×K	933.44	Joback Method
cpg	896.21	J/mol×K	970.09	Joback Method
cpg	907.52	J/mol×K	1006.74	Joback Method
cpg	917.60	J/mol×K	1043.39	Joback Method
cpg	926.47	J/mol×K	1080.04	Joback Method
cpg	934.19	J/mol×K	1116.68	Joback Method
cpg	940.77	J/mol×K	1153.33	Joback Method

Sources

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=U119839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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