Levobunolol, acetylated

Inchi: InChI=1S/C22H31NO4/c1-15(24)23(22(3,4)5)14-18(27-16(2)25)13-12-17-8-6-10-20-19(1
InchiKey: FDNCNNFMRCDNRW-GOSISDBHSA-N
Formula: C22H31NO4
SMILES: CC(=O)OC(CCc1cccc2c1CCCC2=O)CN(C(C)=O)C(C)(C)C
Mol. weight [g/mol]: 373.49

Physical Properties

Property code	Value	Unit	Source
gf	-90.38	kJ/mol	Joback Method
hf	-638.42	kJ/mol	Joback Method
hfus	36.94	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.717		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	961.83	K	Joback Method
tc	1191.16	K	Joback Method
tf	618.02	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.98	J/mol×K	961.83	Joback Method
cpg	1040.30	J/mol×K	1000.05	Joback Method
cpg	1054.30	J/mol×K	1038.27	Joback Method
cpg	1067.06	J/mol×K	1076.49	Joback Method
cpg	1078.65	J/mol×K	1114.72	Joback Method
cpg	1089.17	J/mol×K	1152.94	Joback Method
cpg	1098.69	J/mol×K	1191.16	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=R582662&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

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