Propranolol hydroxy - H2O, isomer II, acetylated

Inchi: InChI=1S/C20H23NO4/c1-14(2)21(15(3)22)12-7-13-24-19-10-11-20(25-16(4)23)18-9-6-5

InchiKey: MVXNVYDTJSLASO-GHXNOFRVSA-N

Formula: C20H23NO4

SMILES: CC(=O)Oc1ccc(OCC=CN(C(C)=O)C(C)C)c2ccccc12

Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
gf	38.04	kJ/mol	Joback Method
hf	-361.60	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	85.28	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	3.914		Crippen Method
mcvol	270.000	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2900.00		NIST Webbook
tb	881.36	K	Joback Method
tc	1102.59	K	Joback Method
tf	556.03	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.67	J/mol×K	881.36	Joback Method
cpg	830.86	J/mol×K	918.23	Joback Method
cpg	844.03	J/mol×K	955.10	Joback Method
cpg	856.24	J/mol×K	991.97	Joback Method
cpg	867.58	J/mol×K	1028.85	Joback Method
cpg	878.10	J/mol×K	1065.72	Joback Method
cpg	887.90	J/mol×K	1102.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583021&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