Oxprenolol hydroxy - H2O, isomer II, acetylated

Inchi: InChI=1S/C20H27NO4/c1-6-13-24-20-11-10-19(25-17(5)23)14-18(20)9-7-8-12-21(15(2)3

InchiKey: ZELDAZQWTKTVKR-BQYQJAHWSA-N

Formula: C20H27NO4

SMILES: C=CCOc1ccc(OC(C)=O)cc1CC=CCN(C(C)=O)C(C)C

Mol. weight [g/mol]: 345.43

Physical Properties

Property code	Value	Unit	Source
gf	19.23	kJ/mol	Joback Method
hf	-427.24	kJ/mol	Joback Method
hfus	44.81	kJ/mol	Joback Method
hvap	82.97	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.532		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	859.06	K	Joback Method
tc	1067.25	K	Joback Method
tf	521.57	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.63	J/mol×K	859.06	Joback Method
cpg	880.89	J/mol×K	893.76	Joback Method
cpg	895.07	J/mol×K	928.46	Joback Method
cpg	908.20	J/mol×K	963.16	Joback Method
cpg	920.33	J/mol×K	997.86	Joback Method
cpg	931.52	J/mol×K	1032.56	Joback Method
cpg	941.79	J/mol×K	1067.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582855&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

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