Oxprenolol, acetylated

Inchi: InChI=1S/C20H29NO4/c1-6-13-24-20-10-8-7-9-18(20)11-12-19(25-17(5)23)14-21(15(2)3
InchiKey: XOARXCAMBBJEOR-UHFFFAOYSA-N
Formula: C20H29NO4
SMILES: C=CCOc1ccccc1CCC(CN(C(C)=O)C(C)C)OC(C)=O
Mol. weight [g/mol]: 347.45

Physical Properties

Property code	Value	Unit	Source
gf	-53.80	kJ/mol	Joback Method
hf	-538.27	kJ/mol	Joback Method
hfus	41.48	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.373		Crippen Method
mcvol	289.460	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	849.48	K	Joback Method
tc	1054.40	K	Joback Method
tf	499.13	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.67	J/mol×K	849.48	Joback Method
cpg	909.59	J/mol×K	883.63	Joback Method
cpg	924.33	J/mol×K	917.79	Joback Method
cpg	937.93	J/mol×K	951.94	Joback Method
cpg	950.43	J/mol×K	986.09	Joback Method
cpg	961.87	J/mol×K	1020.24	Joback Method
cpg	972.27	J/mol×K	1054.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582815&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