Propranolol desamino hydroxy, acetylated

Inchi: InChI=1S/C17H18O5/c1-12(18)20-10-15(22-13(2)19)11-21-17-9-5-7-14-6-3-4-8-16(14)17
InchiKey: FUSSNXRQRFNZPC-UHFFFAOYSA-N
Formula: C17H18O5
SMILES: CC(=O)OCC(COc1cccc2ccccc12)OC(C)=O
Mol. weight [g/mol]: 302.32

Physical Properties

Property code	Value	Unit	Source
gf	-273.59	kJ/mol	Joback Method
hf	-605.18	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	78.35	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.713		Crippen Method
mcvol	227.920	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	813.56	K	Joback Method
tc	1034.09	K	Joback Method
tf	504.54	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.61	J/mol×K	813.56	Joback Method
cpg	674.12	J/mol×K	850.32	Joback Method
cpg	686.53	J/mol×K	887.07	Joback Method
cpg	697.88	J/mol×K	923.83	Joback Method
cpg	708.18	J/mol×K	960.58	Joback Method
cpg	717.47	J/mol×K	997.34	Joback Method
cpg	725.77	J/mol×K	1034.09	Joback Method
dvisc	0.0007203	Pa×s	504.54	Joback Method

dvisc	0.0004558	Pa×s	556.04	Joback Method
dvisc	0.0003117	Pa×s	607.55	Joback Method
dvisc	0.0002262	Pa×s	659.05	Joback Method
dvisc	0.0001720	Pa×s	710.55	Joback Method
dvisc	0.0001357	Pa×s	762.06	Joback Method
dvisc	0.0001103	Pa×s	813.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582984&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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