

Oxprenolol desamino hydroxy, acetylated

Inchi:	InChI=1S/C17H22O5/c1-4-11-20-17-8-6-5-7-15(17)9-10-16(22-14(3)19)12-21-13(2)18/h4
InchiKey:	JBRUEXJSXJGHPC-UHFFFAOYSA-N
Formula:	C17H22O5
SMILES:	<chem>C=CCOc1ccccc1CCC(COC(C)=O)OC(C)=O</chem>
Mol. weight [g/mol]:	306.35

Physical Properties

Property code	Value	Unit	Source
gf	-292.40	kJ/mol	Joback Method
hf	-670.82	kJ/mol	Joback Method
hfus	35.40	kJ/mol	Joback Method
hvap	76.04	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.679		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1900.00		NIST Webbook
tb	791.26	K	Joback Method
tc	996.28	K	Joback Method
tf	470.08	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.13	J/molxK	791.26	Joback Method
cpg	721.82	J/molxK	825.43	Joback Method
cpg	735.44	J/molxK	859.60	Joback Method
cpg	748.01	J/molxK	893.77	Joback Method
cpg	759.52	J/molxK	927.94	Joback Method
cpg	769.98	J/molxK	962.11	Joback Method
cpg	779.41	J/molxK	996.28	Joback Method
dvisc	0.0006419	Paxs	470.08	Joback Method
dvisc	0.0003549	Paxs	523.61	Joback Method

dvisc	0.0002190	Paxs	577.14	Joback Method
dvisc	0.0001467	Paxs	630.67	Joback Method
dvisc	0.0001046	Paxs	684.20	Joback Method
dvisc	0.0000784	Paxs	737.73	Joback Method
dvisc	0.0000610	Paxs	791.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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