

Toliprolol desamino hydroxy, acetylated

Inchi:	InChI=1S/C14H18O5/c1-10-5-4-6-13(7-10)18-9-14(19-12(3)16)8-17-11(2)15/h4-7,14H,8
InchiKey:	YBZAUDYBEYBZHG-UHFFFAOYSA-N
Formula:	C14H18O5
SMILES:	CC(=O)OCC(COc1cccc(C)c1)OC(C)=O
Mol. weight [g/mol]:	266.29

Physical Properties

Property code	Value	Unit	Source
gf	-405.50	kJ/mol	Joback Method
hf	-734.33	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	70.03	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.869		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	725.94	K	Joback Method
tc	933.66	K	Joback Method
tf	438.03	K	Joback Method
vc	0.771	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.18	J/molxK	725.94	Joback Method
cpg	629.17	J/molxK	899.04	Joback Method
cpg	618.70	J/molxK	864.42	Joback Method
cpg	607.26	J/molxK	829.80	Joback Method
cpg	594.85	J/molxK	795.18	Joback Method
cpg	581.49	J/molxK	760.56	Joback Method
cpg	638.67	J/molxK	933.66	Joback Method
dvisc	0.0000849	Paxs	725.94	Joback Method

dvisc	0.0001085	Paxs	677.96	Joback Method
dvisc	0.0001438	Paxs	629.97	Joback Method
dvisc	0.0001996	Paxs	581.99	Joback Method
dvisc	0.0002940	Paxs	534.00	Joback Method
dvisc	0.0004673	Paxs	486.02	Joback Method
dvisc	0.0008224	Paxs	438.03	Joback Method

Sources

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=R583081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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