Nadolol, acetylated

Inchi: InChI=1S/C25H35NO8/c1-15(27)26(25(5,6)7)13-20(32-16(2)28)14-31-22-10-8-9-19-11-2
InchiKey: GHALGKHSFATSNX-BPAKYRGESA-N
Formula: C25H35NO8
SMILES: CC(=O)OC(COc1cccc2c1CC(OC(C)=O)C(OC(C)=O)C2)CN(C(C)=O)C(C)(C)C
Mol. weight [g/mol]: 477.55

Physical Properties

Property code	Value	Unit	Source
gf	-530.79	kJ/mol	Joback Method
hf	-1225.14	kJ/mol	Joback Method
hfus	54.11	kJ/mol	Joback Method
hvap	111.60	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	2.606		Crippen Method
mcvol	368.230	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2650.00		NIST Webbook
tb	1128.31	K	Joback Method
tc	1382.43	K	Joback Method
tf	741.68	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.72	J/mol×K	1128.31	Joback Method
cpg	1295.53	J/mol×K	1170.66	Joback Method
cpg	1303.29	J/mol×K	1213.02	Joback Method
cpg	1309.07	J/mol×K	1255.37	Joback Method
cpg	1312.96	J/mol×K	1297.73	Joback Method
cpg	1315.01	J/mol×K	1340.08	Joback Method
cpg	1315.30	J/mol×K	1382.43	Joback Method

Sources

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=R582786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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