Penbutolol dihydroxy, acetylated

Inchi: InChI=1S/C26H37NO8/c1-16(28)27(26(5,6)7)14-22(34-18(3)30)15-32-25-23(20-10-8-9-1
InchiKey: NPBNHQPXWQDFJA-UHFFFAOYSA-N
Formula: C26H37NO8
SMILES: CC(=O)Oc1cc(OC(C)=O)c(OCC(CN(C(C)=O)C(C)(C)C)OC(C)=O)c(C2CCCC2)c1
Mol. weight [g/mol]: 491.57

Physical Properties

Property code	Value	Unit	Source
gf	-536.39	kJ/mol	Joback Method
hf	-1243.07	kJ/mol	Joback Method
hfus	53.14	kJ/mol	Joback Method
hvap	114.97	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.152		Crippen Method
mcvol	382.320	ml/mol	McGowan Method
pc	1082.78	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	1165.11	K	Joback Method
tc	1429.08	K	Joback Method
tf	766.19	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1339.43	J/mol×K	1165.11	Joback Method
cpg	1347.68	J/mol×K	1209.11	Joback Method
cpg	1353.60	J/mol×K	1253.10	Joback Method
cpg	1357.26	J/mol×K	1297.10	Joback Method
cpg	1358.73	J/mol×K	1341.09	Joback Method
cpg	1358.09	J/mol×K	1385.09	Joback Method
cpg	1355.41	J/mol×K	1429.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582895&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

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