Penbutolol hydroxy, acetylated

Inchi: InChI=1S/C24H35NO6/c1-16(26)25(24(4,5)6)14-21(31-18(3)28)15-29-23-12-11-20(30-17
InchiKey: SJFPHOYVGJCWQJ-UHFFFAOYSA-N
Formula: C24H35NO6
SMILES: CC(=O)Oc1ccc(OCC(CN(C(C)=O)C(C)(C)C)OC(C)=O)c(C2CCCC2)c1
Mol. weight [g/mol]: 433.54

Physical Properties

Property code	Value	Unit	Source
gf	-309.68	kJ/mol	Joback Method
hf	-945.52	kJ/mol	Joback Method
hfus	45.56	kJ/mol	Joback Method
hvap	100.70	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.227		Crippen Method
mcvol	346.700	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2520.00		NIST Webbook
tb	1038.08	K	Joback Method
tc	1272.92	K	Joback Method
tf	658.97	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.60	J/mol×K	1038.08	Joback Method
cpg	1207.12	J/mol×K	1077.22	Joback Method
cpg	1219.00	J/mol×K	1116.36	Joback Method
cpg	1229.31	J/mol×K	1155.50	Joback Method
cpg	1238.13	J/mol×K	1194.64	Joback Method
cpg	1245.53	J/mol×K	1233.78	Joback Method
cpg	1251.58	J/mol×K	1272.92	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=R582904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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