Bunitrolol hydroxy, methoxy, acetylated

Inchi: InChI=1S/C21H28N2O7/c1-13(24)23(21(4,5)6)11-18(30-15(3)26)12-28-20-16(10-22)8-17
InchiKey: XKPFLPMKDIAQKQ-UHFFFAOYSA-N
Formula: C21H28N2O7
SMILES: COc1cc(OC(C)=O)cc(C#N)c1OCC(CN(C(C)=O)C(C)(C)C)OC(C)=O
Mol. weight [g/mol]: 420.46

Physical Properties

Property code	Value	Unit	Source
gf	-352.94	kJ/mol	Joback Method
hf	-922.89	kJ/mol	Joback Method
hfus	46.16	kJ/mol	Joback Method
hvap	107.32	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.450		Crippen Method
mcvol	322.540	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	1083.64	K	Joback Method
tc	1326.68	K	Joback Method
tf	714.00	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.63	J/mol×K	1083.64	Joback Method
cpg	1063.95	J/mol×K	1124.15	Joback Method
cpg	1070.45	J/mol×K	1164.65	Joback Method
cpg	1075.17	J/mol×K	1205.16	Joback Method
cpg	1078.11	J/mol×K	1245.67	Joback Method
cpg	1079.30	J/mol×K	1286.18	Joback Method
cpg	1078.75	J/mol×K	1326.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582548&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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