Metipranolol, desacetyl, acetylated

Inchi: InChI=1S/C21H31NO6/c1-12(2)22(16(6)23)10-19(27-17(7)24)11-26-20-9-13(3)21(28-18(
InchiKey: UVSZIEHVNXXAOV-UHFFFAOYSA-N
Formula: C21H31NO6
SMILES: CC(=O)Oc1c(C)cc(OCC(CN(C(C)=O)C(C)C)OC(C)=O)c(C)c1C
Mol. weight [g/mol]: 393.47

Physical Properties

Property code	Value	Unit	Source
gf	-396.03	kJ/mol	Joback Method
hf	-963.55	kJ/mol	Joback Method
hfus	46.97	kJ/mol	Joback Method
hvap	96.00	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.105		Crippen Method
mcvol	315.290	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	966.91	K	Joback Method
tc	1185.88	K	Joback Method
tf	621.88	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1021.51	J/mol×K	966.91	Joback Method
cpg	1034.90	J/mol×K	1003.40	Joback Method
cpg	1046.73	J/mol×K	1039.90	Joback Method
cpg	1057.01	J/mol×K	1076.39	Joback Method
cpg	1065.75	J/mol×K	1112.89	Joback Method
cpg	1072.94	J/mol×K	1149.38	Joback Method
cpg	1078.59	J/mol×K	1185.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582706&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