Metipranolol desacetyl - H2O, acetylated

Inchi: InChI=1S/C19H27NO4/c1-12(2)20(16(6)21)9-8-10-23-18-11-13(3)19(24-17(7)22)15(5)14
InchiKey: PFZRDNUAGKEPQX-CMDGGOBGSA-N
Formula: C19H27NO4
SMILES: CC(=O)Oc1c(C)cc(OCC=CN(C(C)=O)C(C)C)c(C)c1C
Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
gf	-96.29	kJ/mol	Joback Method
hf	-554.97	kJ/mol	Joback Method
hfus	42.72	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.687		Crippen Method
mcvol	275.370	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2660.00		NIST Webbook
tb	849.46	K	Joback Method
tc	1057.55	K	Joback Method
tf	537.10	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.00	J/mol×K	849.46	Joback Method
cpg	848.37	J/mol×K	884.14	Joback Method
cpg	862.63	J/mol×K	918.82	Joback Method
cpg	875.83	J/mol×K	953.50	Joback Method
cpg	887.99	J/mol×K	988.19	Joback Method
cpg	899.12	J/mol×K	1022.87	Joback Method
cpg	909.26	J/mol×K	1057.55	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=R582711&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