Nordimedrol acetylated

Inchi: InChI=1S/C18H21NO2/c1-15(20)19(2)13-14-21-18(16-9-5-3-6-10-16)17-11-7-4-8-12-17/h
InchiKey: RRLHRDNTUZHNAO-UHFFFAOYSA-N
Formula: C18H21NO2
SMILES: CC(=O)N(C)CCOC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	199.92	kJ/mol	Joback Method
hf	-124.34	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	71.03	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.271		Crippen Method
mcvol	234.380	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2344.00		NIST Webbook
tb	752.89	K	Joback Method
tc	978.58	K	Joback Method
tf	435.09	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.64	J/mol×K	752.89	Joback Method
cpg	684.60	J/mol×K	790.51	Joback Method
cpg	700.25	J/mol×K	828.12	Joback Method
cpg	714.65	J/mol×K	865.74	Joback Method
cpg	727.88	J/mol×K	903.35	Joback Method
cpg	740.01	J/mol×K	940.97	Joback Method
cpg	751.11	J/mol×K	978.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R593370&Units=SI

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