Nifenalol, diacetyl deriv.

Other names: Nifenalol, acetylated
Inchi: InChI=1S/C15H20N2O5/c1-10(2)16(11(3)18)9-15(22-12(4)19)13-5-7-14(8-6-13)17(20)21
InchiKey: ODKUBEOVIIEYQB-UHFFFAOYSA-N
Formula: C15H20N2O5
SMILES: CC(=O)OC(CN(C(C)=O)C(C)C)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 308.33

Physical Properties

Property code	Value	Unit	Source
gf	-43.19	kJ/mol	Joback Method
hf	-439.04	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	85.68	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.456		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	867.82	K	Joback Method
tc	1096.65	K	Joback Method
tf	565.92	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.06	J/mol×K	867.82	Joback Method
cpg	726.82	J/mol×K	905.96	Joback Method
cpg	738.44	J/mol×K	944.10	Joback Method
cpg	748.96	J/mol×K	982.24	Joback Method
cpg	758.44	J/mol×K	1020.38	Joback Method
cpg	766.91	J/mol×K	1058.52	Joback Method
cpg	774.45	J/mol×K	1096.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U280821&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