

Nifenalol - H2O, acetylated

Inchi:	InChI=1S/C13H16N2O3/c1-10(2)14(11(3)16)9-8-12-4-6-13(7-5-12)15(17)18/h4-10H,1-3H
InchiKey:	XQKVOHRMNADECP-CMDGGOBGSA-N
Formula:	C13H16N2O3
SMILES:	CC(=O)N(C=Cc1ccc([N+](=O)[O-])cc1)C(C)C
Mol. weight [g/mol]:	248.28

Physical Properties

Property code	Value	Unit	Source
gf	256.55	kJ/mol	Joback Method
hf	-30.46	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.822		Crippen Method
mcvol	194.940	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	2265.00		NIST Webbook
rinpol	2265.00		NIST Webbook
tb	750.37	K	Joback Method
tc	987.12	K	Joback Method
tf	481.14	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.90	J/molxK	750.37	Joback Method
cpg	553.73	J/molxK	789.83	Joback Method
cpg	566.50	J/molxK	829.29	Joback Method
cpg	578.29	J/molxK	868.74	Joback Method
cpg	589.21	J/molxK	908.20	Joback Method
cpg	599.33	J/molxK	947.66	Joback Method
cpg	608.74	J/molxK	987.12	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=R582800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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