Bunitrolol, acetylated

Inchi: InChI=1S/C18H24N2O4/c1-13(21)20(18(3,4)5)11-16(24-14(2)22)12-23-17-9-7-6-8-15(17
InchiKey: KJGVBWDSAUYHCJ-UHFFFAOYSA-N
Formula: C18H24N2O4
SMILES: CC(=O)OC(COc1ccccc1C#N)CN(C(C)=O)C(C)(C)C
Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	-20.02	kJ/mol	Joback Method
hf	-461.01	kJ/mol	Joback Method
hfus	35.19	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.516		Crippen Method
mcvol	266.960	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	2070.00		NIST Webbook
tb	906.33	K	Joback Method
tc	1127.41	K	Joback Method
tf	560.76	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.74	J/mol×K	906.33	Joback Method
cpg	840.48	J/mol×K	943.18	Joback Method
cpg	852.10	J/mol×K	980.02	Joback Method
cpg	862.66	J/mol×K	1016.87	Joback Method
cpg	872.20	J/mol×K	1053.72	Joback Method
cpg	880.79	J/mol×K	1090.57	Joback Method
cpg	888.47	J/mol×K	1127.41	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=R582513&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

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