Nortropin, 1-hydroxy-3-«beta»-benzoyl

Inchi: InChI=1S/C14H17NO3/c16-13(10-4-2-1-3-5-10)18-12-8-11-6-7-14(17,9-12)15-11/h1-5,11
InchiKey: LNUWTPXKDUMTGP-YRGRVCCFSA-N
Formula: C14H17NO3
SMILES: O=C(OC1CC2CCC(O)(C1)N2)c1ccccc1
Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
gf	-19.52	kJ/mol	Joback Method
hf	-326.80	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	1.446		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	2948.00		NIST Webbook
tb	781.01	K	Joback Method
tc	1014.50	K	Joback Method
tf	560.47	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.27	J/mol×K	781.01	Joback Method
cpg	589.95	J/mol×K	819.92	Joback Method
cpg	605.03	J/mol×K	858.84	Joback Method
cpg	619.69	J/mol×K	897.75	Joback Method
cpg	634.11	J/mol×K	936.67	Joback Method
cpg	648.46	J/mol×K	975.58	Joback Method
cpg	662.92	J/mol×K	1014.50	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=R578039&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