3-(Hydroxybenzoyloxy)nortropane

Inchi: InChI=1S/C14H17NO3/c16-12-5-1-9(2-6-12)14(17)18-13-7-10-3-4-11(8-13)15-10/h1-2,5-
InchiKey: DWQUGXKAGSBTHT-QYJAPNMZSA-N
Formula: C14H17NO3
SMILES: O=C(OC1CC2CCC(C1)N2)c1ccc(O)cc1
Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
gf	-31.83	kJ/mol	Joback Method
hf	-367.12	kJ/mol	Joback Method
hfus	37.36	kJ/mol	Joback Method
hvap	77.82	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	1.832		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	2290.00		NIST Webbook
tb	769.21	K	Joback Method
tc	1021.60	K	Joback Method
tf	587.47	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.30	J/mol×K	769.21	Joback Method
cpg	591.87	J/mol×K	811.27	Joback Method
cpg	607.26	J/mol×K	853.34	Joback Method
cpg	621.64	J/mol×K	895.40	Joback Method
cpg	635.15	J/mol×K	937.47	Joback Method
cpg	647.93	J/mol×K	979.53	Joback Method
cpg	660.13	J/mol×K	1021.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R509810&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

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