3-(Hydroxypentanoyloxy)nortropane

Inchi: InChI=1S/C12H21NO3/c1-2-3-11(14)12(15)16-10-6-8-4-5-9(7-10)13-8/h8-11,13-14H,2-7
InchiKey: JZUPZKQOYGESCW-IXBNRNDTSA-N
Formula: C12H21NO3
SMILES: CCCC(O)C(=O)OC1CC2CCC(C1)N2
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-145.72	kJ/mol	Joback Method
hf	-542.57	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	74.37	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	0.974		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1603.00		NIST Webbook
tb	707.89	K	Joback Method
tc	909.29	K	Joback Method
tf	472.61	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.57	J/mol×K	707.89	Joback Method
cpg	573.38	J/mol×K	741.46	Joback Method
cpg	588.25	J/mol×K	775.02	Joback Method
cpg	602.20	J/mol×K	808.59	Joback Method
cpg	615.28	J/mol×K	842.16	Joback Method
cpg	627.51	J/mol×K	875.72	Joback Method
cpg	638.94	J/mol×K	909.29	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=R509830&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