6-Pentanoyloxynortropan-6-ol

Inchi: InChI=1S/C12H21NO3/c1-2-3-4-12(15)16-11-6-8-5-9(14)7-10(11)13-8/h8-11,13-14H,2-7
InchiKey: VFRBSLVVGKTPQL-QPBDYMMBSA-N
Formula: C12H21NO3
SMILES: CCCCC(=O)OC1CC2CC(O)CC1N2
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-150.99	kJ/mol	Joback Method
hf	-557.63	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	74.45	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	0.974		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1719.00		NIST Webbook
tb	703.66	K	Joback Method
tc	901.75	K	Joback Method
tf	483.37	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.70	J/mol×K	703.66	Joback Method
cpg	575.67	J/mol×K	736.68	Joback Method
cpg	590.72	J/mol×K	769.69	Joback Method
cpg	604.86	J/mol×K	802.71	Joback Method
cpg	618.14	J/mol×K	835.72	Joback Method
cpg	630.57	J/mol×K	868.74	Joback Method
cpg	642.19	J/mol×K	901.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R509989&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