4-(cis-3-hexenoxy)-«gamma»-valerolactone

Inchi: InChI=1S/C11H18O3/c1-3-4-5-6-7-13-10-8-11(12)14-9(10)2/h4-5,9-10H,3,6-8H2,1-2H3/b
InchiKey: IBAKBAAEJZENMM-PLNGDYQASA-N
Formula: C11H18O3
SMILES: CCC=CCCOC1CC(=O)OC1C
Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
gf	-162.91	kJ/mol	Joback Method
hf	-514.93	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	51.15	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.063		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
ripol	2114.00		NIST Webbook
tb	583.04	K	Joback Method
tc	791.04	K	Joback Method
tf	332.33	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.69	J/mol×K	583.04	Joback Method
cpg	446.29	J/mol×K	617.71	Joback Method
cpg	463.02	J/mol×K	652.37	Joback Method
cpg	478.89	J/mol×K	687.04	Joback Method
cpg	493.91	J/mol×K	721.71	Joback Method
cpg	508.06	J/mol×K	756.37	Joback Method
cpg	521.36	J/mol×K	791.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321412&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume