4-Hydroxy-nonadecanoic, «gamma»-lactone

Inchi: InChI=1S/C19H36O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16-17-19(20)21-18/h18H
InchiKey: WTNURYXISAYHFJ-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: CCCCCCCCCCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 296.49

Physical Properties

Property code	Value	Unit	Source
gf	-63.06	kJ/mol	Joback Method
hf	-644.71	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.173		Crippen Method
mcvol	275.150	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	2294.00		NIST Webbook
tb	744.17	K	Joback Method
tc	931.36	K	Joback Method
tf	409.58	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.23	J/mol×K	744.17	Joback Method
cpg	883.91	J/mol×K	775.37	Joback Method
cpg	903.48	J/mol×K	806.57	Joback Method
cpg	921.96	J/mol×K	837.77	Joback Method
cpg	939.39	J/mol×K	868.97	Joback Method
cpg	955.77	J/mol×K	900.17	Joback Method
cpg	971.14	J/mol×K	931.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R186917&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume