

5-Hydroxy-nonadecanoic, «delta»-lactone

Inchi:	InChI=1S/C19H36O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-16-14-17-19(20)21-18/h18H
InchiKey:	XIAPRFCGBMILCN-UHFFFAOYSA-N
Formula:	C19H36O2
SMILES:	CCCCCCCCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	296.49

Physical Properties

Property code	Value	Unit	Source
gf	-75.16	kJ/mol	Joback Method
hf	-650.87	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	67.07	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.173		Crippen Method
mcvol	275.150	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	748.44	K	Joback Method
tc	939.59	K	Joback Method
tf	406.06	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.27	J/mol×K	748.44	Joback Method
cpg	888.51	J/mol×K	780.30	Joback Method
cpg	908.54	J/mol×K	812.16	Joback Method
cpg	927.39	J/mol×K	844.02	Joback Method
cpg	945.08	J/mol×K	875.88	Joback Method
cpg	961.63	J/mol×K	907.73	Joback Method
cpg	977.05	J/mol×K	939.59	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=R186868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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