4-Hydroxy-heptadecanoic acid, «gamma»-lactone

Inchi: InChI=1S/C17H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-14-15-17(18)19-16/h16H,2-15H

InchiKey: ZZKHCCCWEVWBPD-UHFFFAOYSA-N

Formula: C17H32O2

SMILES: CCCCCCCCCCCCCCC1CCC(=O)O1

Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-79.90	kJ/mol	Joback Method
hf	-603.43	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	62.45	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.393		Crippen Method
mcvol	246.970	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	2098.00		NIST Webbook
tb	698.41	K	Joback Method
tc	886.87	K	Joback Method
tf	387.04	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.91	J/mol×K	698.41	Joback Method
cpg	765.18	J/mol×K	729.82	Joback Method
cpg	784.41	J/mol×K	761.23	Joback Method
cpg	802.60	J/mol×K	792.64	Joback Method
cpg	819.78	J/mol×K	824.05	Joback Method
cpg	835.98	J/mol×K	855.46	Joback Method
cpg	851.20	J/mol×K	886.87	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=R186808&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