5-Hydroxy-heptadecanoic acid, «delta»-lactone

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

InchiKey: SNHVOIJTSDIHOA-UHFFFAOYSA-N

Formula: C17H32O2

SMILES: CCCCCCCCCCCCC1CCCC(=O)O1

Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-92.00	kJ/mol	Joback Method
hf	-609.59	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	62.62	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.393		Crippen Method
mcvol	246.970	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	702.68	K	Joback Method
tc	895.85	K	Joback Method
tf	383.52	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.40	J/mol×K	702.68	Joback Method
cpg	769.36	J/mol×K	734.88	Joback Method
cpg	789.19	J/mol×K	767.07	Joback Method
cpg	807.89	J/mol×K	799.27	Joback Method
cpg	825.48	J/mol×K	831.46	Joback Method
cpg	841.98	J/mol×K	863.66	Joback Method
cpg	857.40	J/mol×K	895.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R186759&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