4-Hydroxy-arachidic, «gamma»-lactone

Inchi: InChI=1S/C20H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-17-18-20(21)22-19/h1
InchiKey: OIAOPTWTWLRDHD-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: CCCCCCCCCCCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 310.51

Physical Properties

Property code	Value	Unit	Source
gf	-54.64	kJ/mol	Joback Method
hf	-665.35	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.563		Crippen Method
mcvol	289.240	ml/mol	McGowan Method
pc	1163.25	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	767.05	K	Joback Method
tc	954.40	K	Joback Method
tf	420.85	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.83	J/mol×K	767.05	Joback Method
cpg	944.70	J/mol×K	798.28	Joback Method
cpg	964.43	J/mol×K	829.50	Joback Method
cpg	983.03	J/mol×K	860.73	Joback Method
cpg	1000.55	J/mol×K	891.95	Joback Method
cpg	1017.00	J/mol×K	923.18	Joback Method
cpg	1032.41	J/mol×K	954.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R186937&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