(Z)-18-Octadec-9-enolide

Inchi: InChI=1S/C18H32O2/c19-18-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-17-20-18/h1-2H,3-
InchiKey: GODWWTDBDJRXIU-UPHRSURJSA-N
Formula: C18H32O2
SMILES: O=C1CCCCCCCC=CCCCCCCCCO1
Mol. weight [g/mol]: 280.45
CAS: 80060-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-203.21	kJ/mol	Joback Method
hf	-632.19	kJ/mol	Joback Method
hfus	14.55	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.561		Crippen Method
mcvol	256.760	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2158.90		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2158.90		NIST Webbook
tb	784.90	K	Joback Method
tc	1061.28	K	Joback Method
tf	354.03	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.75	J/mol×K	784.90	Joback Method
cpg	862.15	J/mol×K	830.96	Joback Method
cpg	887.81	J/mol×K	877.03	Joback Method
cpg	909.59	J/mol×K	923.09	Joback Method
cpg	927.32	J/mol×K	969.15	Joback Method

cpg	940.86	J/mol×K	1015.22	Joback Method
cpg	950.04	J/mol×K	1061.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80060760&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