10-Oxahexadecanolide

Inchi: InChI=1S/C16H30O2/c1-2-3-4-9-12-15-13-10-7-5-6-8-11-14-16(17)18-15/h15H,2-14H2,1
InchiKey: DNJTZERFZIMFQV-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CCCCCCC1CCCCCCCCC(=O)O1
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
gf	-160.92	kJ/mol	Joback Method
hf	-619.75	kJ/mol	Joback Method
hfus	26.02	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.003		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1904.50		NIST Webbook
rinpol	1904.50		NIST Webbook
tb	701.15	K	Joback Method
tc	925.59	K	Joback Method
tf	354.65	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.58	J/mol×K	701.15	Joback Method
cpg	732.58	J/mol×K	738.56	Joback Method
cpg	755.84	J/mol×K	775.96	Joback Method
cpg	777.35	J/mol×K	813.37	Joback Method
cpg	797.06	J/mol×K	850.78	Joback Method
cpg	814.96	J/mol×K	888.19	Joback Method
cpg	831.03	J/mol×K	925.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R185107&Units=SI

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