14-Methylpentadecano-15-lactone

Inchi: InChI=1S/C16H30O2/c1-15-12-10-8-6-4-2-3-5-7-9-11-13-16(17)18-14-15/h15H,2-14H2,1
InchiKey: BXUAFPXADZNGNU-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CC1CCCCCCCCCCCCC(=O)OC1
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
gf	-221.42	kJ/mol	Joback Method
hf	-650.55	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.861		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1877.00		NIST Webbook
rinpol	1877.00		NIST Webbook
ripol	2253.00		NIST Webbook
ripol	2253.00		NIST Webbook
tb	722.50	K	Joback Method
tc	984.52	K	Joback Method
tf	337.05	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.50	J/mol×K	722.50	Joback Method
cpg	756.49	J/mol×K	766.17	Joback Method
cpg	783.67	J/mol×K	809.84	Joback Method
cpg	807.91	J/mol×K	853.51	Joback Method
cpg	829.10	J/mol×K	897.18	Joback Method
cpg	847.13	J/mol×K	940.85	Joback Method

cpg	861.88	J/mol×K	984.52	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=R341114&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume