Oxacycloheptadecan-2-one

Other names:	Cyclohexadecanolide
	Dihydroambrettolide
	Hexadecanoic acid, 16-hydroxy-, «omicron»-lactone
	Hexadecanolide
	Juniperic acid lactone
	1,16-Hexadecanolide
	16-Hexadecanolactone
	16-Hexadecanolide
	1,16-Hexadecanolactone
	16-Hydroxyhexadecanoic acid lactone
	Hexadecano-16-lactone
	NSC 33546
	Oxa-2-cycloheptadecanone
Inchi:	InChI=1S/C16H30O2/c17-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-18-16/h1-15H2
InchiKey:	LOKPJYNMYCVCRM-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	O=C1CCCCCCCCCCCCCCCO1
Mol. weight [g/mol]:	254.41
CAS:	109-29-5

Physical Properties

Property code	Value	Unit	Source
gf	-225.81	kJ/mol	Joback Method
hf	-636.37	kJ/mol	Joback Method
hfus	12.35	kJ/mol	Joback Method
hvap	62.60	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.005		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1942.00		NIST Webbook
ripol	2334.00		NIST Webbook

ripol	2367.00		NIST Webbook
tb	731.44	K	Joback Method
tc	1001.71	K	Joback Method
tf	337.77	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.67	J/mol×K	731.44	Joback Method
cpg	758.99	J/mol×K	776.48	Joback Method
cpg	786.24	J/mol×K	821.53	Joback Method
cpg	810.28	J/mol×K	866.57	Joback Method
cpg	830.98	J/mol×K	911.62	Joback Method
cpg	848.22	J/mol×K	956.66	Joback Method
cpg	861.87	J/mol×K	1001.71	Joback Method
hvapt	71.60	kJ/mol	433.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109295&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
hvapt: Enthalpy of vaporization at a given temperature
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