Oxacyclohexadecan-2-one

Other names:	1,15-pentadecanolide 15-Hydroxypentadecanoic acid, lactone 15-Pentadecanolactone 15-Pentadecanolide 15-hydroxypentadecanoic acid, .epsilon.-lactone 15-hydroxypentanoic acid, cyclic ester 2-Pentadecalone Cyclopentadecanolactone Muskolactone NSC 36763 Pentadecan-15-olide Pentadecano-15-lactone Pentadecanoic acid, 15-hydroxy-, «xi»-lactone Pentadecanolactone Pentalide cyclopentadecanolide exaltolide muskalactone pentadecalactone pentadecanolide thibetolide
Inchi:	InChI=1S/C15H28O2/c16-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-17-15/h1-14H2
InchiKey:	FKUPPRZPSYCDRS-UHFFFAOYSA-N
Formula:	C15H28O2
SMILES:	O=C1CCCCCCCCCCCCCCO1
Mol. weight [g/mol]:	240.38
CAS:	106-02-5

Physical Properties

Property code	Value	Unit	Source
chs	-9178.10 ± 8.80	kJ/mol	NIST Webbook
chs	-9196.00 ± 4.00	kJ/mol	NIST Webbook
gf	-222.13	kJ/mol	Joback Method
hf	-609.57	kJ/mol	Joback Method
hfs	-725.50 ± 9.00	kJ/mol	NIST Webbook
hfs	-709.00 ± 4.00	kJ/mol	NIST Webbook

hfus	11.86	kJ/mol	Joback Method
hvap	60.20	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.615		Crippen Method
mcvol	218.790	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1840.60		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1840.60		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2242.00		NIST Webbook
ripol	2233.00		NIST Webbook
ss	482.90	J/mol×K	NIST Webbook
ss	482.80	J/mol×K	NIST Webbook
tb	704.29	K	Joback Method
tc	972.50	K	Joback Method
tf	310.20 ± 1.00	K	NIST Webbook
tf	310.15 ± 0.60	K	NIST Webbook
tt	308.50 ± 0.10	K	NIST Webbook
tt	308.50 ± 1.00	K	NIST Webbook
tt	308.50 ± 0.10	K	NIST Webbook
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.06	J/mol×K	793.69	Joback Method
cpg	746.28	J/mol×K	838.39	Joback Method
cpg	767.52	J/mol×K	883.09	Joback Method
cpg	785.64	J/mol×K	927.80	Joback Method

cpg	665.09	J/mol×K	704.29	Joback Method
cpg	694.96	J/mol×K	748.99	Joback Method
cpg	800.54	J/mol×K	972.50	Joback Method
cps	444.30	J/mol×K	298.15	NIST Webbook
cps	444.60	J/mol×K	298.15	NIST Webbook
hfust	6.99	kJ/mol	308.50	NIST Webbook
hfust	27.30	kJ/mol	283.00	NIST Webbook
hfust	6.99	kJ/mol	190.00	NIST Webbook
hsubt	81.30	kJ/mol	300.00	NIST Webbook
hvapt	74.20	kJ/mol	315.00	NIST Webbook
hvapt	78.20	kJ/mol	403.00	NIST Webbook
sfust	22.65	J/mol×K	308.50	NIST Webbook
sfust	96.47	J/mol×K	283.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
High-pressure phase equilibrium data for systems containing carbon dioxide, omega-pentadecalactone, chloroform and water:	https://www.doi.org/10.1016/j.jct.2018.03.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume