Oxacyclotetradecan-2-one

Other names:	Tridecanoic acid, 13-hydroxy-, «mu»-lactone
	Tridecanolide
	1,13-Tridecanolide
	1-Oxacyclotetradecan-2-one
	13-Tridecanolide
	Tridecano-13-lactone
Inchi:	InChI=1S/C13H24O2/c14-13-11-9-7-5-3-1-2-4-6-8-10-12-15-13/h1-12H2
InchiKey:	IUDIJIVSWGWJNV-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	O=C1CCCCCCCCCCCCO1
Mol. weight [g/mol]:	212.33
CAS:	1725-04-8

Physical Properties

Property code	Value	Unit	Source
chs	-7895.30 ± 2.90	kJ/mol	NIST Webbook
gf	-214.77	kJ/mol	Joback Method
hf	-569.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-644.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-648.10 ± 2.90	kJ/mol	NIST Webbook
hfus	10.88	kJ/mol	Joback Method
hvap	72.90 ± 1.70	kJ/mol	NIST Webbook
hvap	75.00	kJ/mol	NIST Webbook
log10ws	-4.02		Crippen Method
logp	3.834		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1640.80		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1636.00		NIST Webbook
ripol	2082.00		NIST Webbook
ripol	2082.00		NIST Webbook
ripol	2062.00		NIST Webbook
ripol	2055.00		NIST Webbook

ripol	2030.00		NIST Webbook
ripol	2030.00		NIST Webbook
ss	401.90	J/mol×K	NIST Webbook
ss	401.80	J/mol×K	NIST Webbook
tb	649.99	K	Joback Method
tc	913.37	K	Joback Method
tf	314.52	K	Joback Method
tt	300.42 ± 0.01	K	NIST Webbook
tt	300.40 ± 0.10	K	NIST Webbook
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.58	J/mol×K	781.68	Joback Method
cpg	641.85	J/mol×K	825.58	Joback Method
cpg	660.68	J/mol×K	869.48	Joback Method
cpg	542.95	J/mol×K	649.99	Joback Method
cpg	571.03	J/mol×K	693.89	Joback Method
cpg	596.94	J/mol×K	737.78	Joback Method
cpg	676.97	J/mol×K	913.37	Joback Method
cps	398.30	J/mol×K	298.15	NIST Webbook
cps	398.30	J/mol×K	298.15	NIST Webbook
hfust	9.08	kJ/mol	300.40	NIST Webbook
hvapt	66.60 ± 1.10	kJ/mol	390.00	NIST Webbook
hvapt	67.50	kJ/mol	418.00	NIST Webbook

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=C1725048&Units=SI

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
hfl:	Liquid phase 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
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
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