

Oxacyclotetradecan-2-one, 13-methyl-

Other names:	12-Methyltridecano-13-lactone
Inchi:	InChI=1S/C14H26O2/c1-13-10-8-6-4-2-3-5-7-9-11-14(15)16-12-13/h13H,2-12H2,1H3
InchiKey:	NFNWPPOMMYDNFQ-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CC1CCCCCCCCCCCCC(=O)OC1
Mol. weight [g/mol]:	226.35
CAS:	57092-32-7

Physical Properties

Property code	Value	Unit	Source
gf	-214.06	kJ/mol	Joback Method
hf	-596.95	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.080		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1681.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2067.00		NIST Webbook
tb	668.20	K	Joback Method
tc	925.56	K	Joback Method
tf	321.55	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.26	J/mol×K	668.20	Joback Method
cpg	629.85	J/mol×K	711.09	Joback Method
cpg	656.21	J/mol×K	753.99	Joback Method
cpg	680.23	J/mol×K	796.88	Joback Method

cpg	701.84	J/mol×K	839.77	Joback Method
cpg	720.93	J/mol×K	882.67	Joback Method
cpg	737.41	J/mol×K	925.56	Joback Method

Sources

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=C57092327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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