

Oxacyclotridecan-2-one

Other names:	Dodecanolactone
Inchi:	InChI=1S/C12H22O2/c13-12-10-8-6-4-2-1-3-5-7-9-11-14-12/h1-11H2
InchiKey:	DQGSJTVMODPFBK-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	O=C1CCCCCCCCCCCCO1
Mol. weight [g/mol]:	198.30
CAS:	947-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-211.09	kJ/mol	Joback Method
hf	-540.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-611.00 ± 3.00	kJ/mol	NIST Webbook
hfus	10.39	kJ/mol	Joback Method
hvap	71.00 ± 1.00	kJ/mol	NIST Webbook
hvap	71.00	kJ/mol	NIST Webbook
hvap	70.50 ± 1.70	kJ/mol	NIST Webbook
log10ws	-3.60		Crippen Method
logp	3.444		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	622.84	K	Joback Method
tc	883.40	K	Joback Method
tf	306.77	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.83	J/mol×K	622.84	Joback Method
cpg	511.62	J/mol×K	666.27	Joback Method
cpg	536.50	J/mol×K	709.69	Joback Method
cpg	559.40	J/mol×K	753.12	Joback Method
cpg	580.23	J/mol×K	796.55	Joback Method

cpg	598.91	J/mol×K	839.97	Joback Method
cpg	615.37	J/mol×K	883.40	Joback Method
hvapt	64.20 ± 1.10	kJ/mol	390.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C947057&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
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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