

Oxacyclododecan-2-one

Other names:	11-Hydroxyundecanoic acid, lactone
Inchi:	InChI=1S/C11H20O2/c12-11-9-7-5-3-1-2-4-6-8-10-13-11/h1-10H2
InchiKey:	MVOSYKNQRRHGKX-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	O=C1CCCCCCCCCCC1
Mol. weight [g/mol]:	184.28
CAS:	1725-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-207.41	kJ/mol	Joback Method
hf	-517.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-583.00 ± 2.00	kJ/mol	NIST Webbook
hfus	9.90	kJ/mol	Joback Method
hvap	66.00 ± 1.00	kJ/mol	NIST Webbook
hvap	66.00	kJ/mol	NIST Webbook
hvap	66.20 ± 1.30	kJ/mol	NIST Webbook
log10ws	-3.18		Crippen Method
logp	3.054		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	595.69	K	Joback Method
tc	853.10	K	Joback Method
tf	299.02	K	Joback Method
tt	275.33 ± 0.01	K	NIST Webbook
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.69	J/mol×K	724.40	Joback Method
cpg	519.77	J/mol×K	767.30	Joback Method
cpg	538.00	J/mol×K	810.20	Joback Method
cpg	428.95	J/mol×K	595.69	Joback Method

cpg	454.21	J/mol×K	638.59	Joback Method
cpg	477.81	J/mol×K	681.49	Joback Method
cpg	554.30	J/mol×K	853.10	Joback Method
hfust	12.61	kJ/mol	275.30	NIST Webbook
hvapt	57.70 ± 0.80	kJ/mol	376.00	NIST Webbook
hvapt	70.50	kJ/mol	383.00	NIST Webbook

Sources

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=C1725037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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