2H-Pyran-2-one, 6-hexyltetrahydro-

Other names:	.delta.-hexylvalerolactone
	.delta.-undecalactone
	.delta.-undecanolactone
	2H-Pyran-2-one, tetrahydro-3-hexyl-
	5-Hydroxy-n-undecanoic acid «delta»-lactone
	5-Hydroxyundecanoic acid lactone
	5-Undecanolide
	6-hexyltetrahydro-2H-pyran-2-one
	Undecan-5-olide
	Undecanoic acid, 5-hydroxy-, «delta»-lactone
	Undecanolactone
	Undecanolide-1,5
	«delta»-Hexyl-«delta»-valerolactone
	«delta»-Hexylvalerolactone
	«delta»-Undecalactone
	«delta»-Undecanolide
Inchi:	InChI=1S/C11H20O2/c1-2-3-4-5-7-10-8-6-9-11(12)13-10/h10H,2-9H2,1H3
InchiKey:	YZRXRLLRSPQHDK-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	184.28
CAS:	710-04-3

Physical Properties

Property code	Value	Unit	Source
gf	-142.52	kJ/mol	Joback Method
hf	-485.75	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.053		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1539.00		NIST Webbook

ripol	2356.00		NIST Webbook
ripol	2345.00		NIST Webbook
ripol	2345.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2336.00		NIST Webbook
sl	369.50	J/mol×K	NIST Webbook
sl	369.50	J/mol×K	NIST Webbook
tb	565.40	K	Joback Method
tc	773.82	K	Joback Method
tf	315.90	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.35	J/mol×K	669.61	Joback Method
cpg	490.47	J/mol×K	704.34	Joback Method
cpg	505.66	J/mol×K	739.08	Joback Method
cpg	420.46	J/mol×K	565.40	Joback Method
cpg	439.35	J/mol×K	600.14	Joback Method
cpg	457.31	J/mol×K	634.87	Joback Method
cpg	519.94	J/mol×K	773.82	Joback Method
cpl	342.70	J/mol×K	298.15	NIST Webbook
cpl	342.70	J/mol×K	298.15	NIST Webbook
hvapt	80.10	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.70	K	1.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta. lactones by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2014.01.016
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=C710043&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume