2(3H)-Furanone, 5-heptyldihydro-

Other names:
.gamma.-heptylbutyrolactone
.gamma.-undecalactone
.gamma.-undecanolactone
1,4-Undecanolide
4-Hydroxyundecanoic acid lactone
4-Hydroxyundecanoic acid, «gamma»-lactone
4-Undecanolide
5-heptyldihydro-2(3H)-furanone
Aldehyde C-14
Aldehyde C-14 peach
NSC 406421
Peach aldehyde
Peach lactone
Persicol
Undecanoic acid, 4-hydroxy-, «gamma»-lactone
Undecanoic «gamma»-lactone
Undecanolide-1,4
undecan-4-olide
«gamma»-Heptyl-«gamma»-butyrolactone
«gamma»-Heptylbutyrolactone
«gamma»-Undecalactone
«gamma»-Undecalatone
«gamma»-Undecanolactone
«gamma»-Undecanolide
«gamma»-Undekalakton
«gamma»-n-Heptylbutyrolactone

Inchi: InChI=1S/C11H20O2/c1-2-3-4-5-6-7-10-8-9-11(12)13-10/h10H,2-9H2,1H3
InchiKey: PHXATPHONSXBIL-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 184.28
CAS: 104-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-130.42	kJ/mol	Joback Method

hf	-479.59	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	49.09	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.053		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1523.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1525.10		NIST Webbook
rinpol	1524.50		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1525.10		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1532.60		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1529.00		NIST Webbook
ripol	2254.70		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2218.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2288.00		NIST Webbook
ripol	2235.00		NIST Webbook

ripol	2270.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2259.30		NIST Webbook
ripol	2238.00		NIST Webbook
tb	561.13	K	Joback Method
tc	762.60	K	Joback Method
tf	319.42	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.25	J/mol×K	561.13	Joback Method
cpg	437.17	J/mol×K	594.71	Joback Method
cpg	454.23	J/mol×K	628.29	Joback Method
cpg	470.45	J/mol×K	661.87	Joback Method
cpg	485.84	J/mol×K	695.45	Joback Method
cpg	500.40	J/mol×K	729.02	Joback Method
cpg	514.15	J/mol×K	762.60	Joback Method
hvapt	79.40	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	438.20	K	1.70	NIST Webbook

Sources

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=C104676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume