«gamma»-Dodecalactone

Other names:	(.+/-.)-4-n-Octylbutyrolactone
	.gamma.-dodecalactone
	.gamma.-dodecanolactone
	.gamma.-laurolactone
	.gamma.-octylbutyrolactone
	2(3H)-Furanone, dihydro-5-octyl-
	2-(3H)-Furanone, 5-octyldihydro-
	4-Dodecanolide
	4-Hydroxydodecanoic acid lactone
	4-Hydroxydodecanoic acid, «gamma»-lactone
	5-octyldihydro-2(3H)-furanone
	Dihydro-5-octyl-2(3H)-furanone
	Dodecan-4-olide
	Dodecanoic acid, 4-hydroxy-, «gamma»-lactone
	Dodecanolide-1,4
	NSC 26511
	dihydro-5-octylfuran-2(3H)-one
	«gamma»-Dodecanolactone
	«gamma»-Dodecanolide
	«gamma»-Octyl-«gamma»-butyrolactone
	«gamma»-n-Octyl-«gamma»-n-butyrolactone
Inchi:	InChI=1S/C12H22O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h11H,2-10H2,1H3
InchiKey:	WGPCZPLRVAWXPW-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]:	198.30
CAS:	2305-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-122.00	kJ/mol	Joback Method
hf	-500.23	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.443		Crippen Method

mcvol	176.520	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1627.30		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1677.00		NIST Webbook
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rinpol	1698.00		NIST Webbook
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ripol	2345.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2379.00		NIST Webbook
ripol	2381.00		NIST Webbook
ripol	2379.00		NIST Webbook
tb	584.01	K	Joback Method
tc	782.64	K	Joback Method
tf	330.69	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.64	J/mol×K	749.53	Joback Method
cpg	469.94	J/mol×K	584.01	Joback Method
cpg	488.44	J/mol×K	617.11	Joback Method
cpg	506.05	J/mol×K	650.22	Joback Method
cpg	522.78	J/mol×K	683.32	Joback Method

cpg	538.64	J/mol×K	716.43	Joback Method
cpg	567.79	J/mol×K	782.64	Joback Method
hvapt	83.90	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography

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=C2305057&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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