«delta»-Dodecalactone

Other names:	.delta.-dodecalactone
	.delta.-dodecanolactone
	.delta.-heptylvalerolactone
	2H-Pyran-2-one, 6-heptyltetrahydro-
	2H-Pyran-2-one, tetrahydro-6-heptyl
	5-Dodecanolide
	5-Hydroxydodecanoic acid lactone
	5-Hydroxydodecanoic acid, «delta»-lactone
	6-heptyltetrahydro-2H-pyran-2-one
	Dodecan-5-olide
	Dodecanoic acid, 5-hydroxy-, «delta»-lactone
	n-Heptyl-«delta»-valerolactone
	«beta»-Dodecalactone
	«delta»-Dodecanolide
	«delta»-Heptyl-«delta»-valerolactone
Inchi:	InChI=1S/C12H22O2/c1-2-3-4-5-6-8-11-9-7-10-12(13)14-11/h11H,2-10H2,1H3
InchiKey:	QRPLZGZHJABGRS-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	198.30
CAS:	713-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-134.10	kJ/mol	Joback Method
hf	-506.39	kJ/mol	Joback Method
hfus	26.16	kJ/mol	Joback Method
hvap	51.49	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.443		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1720.00		NIST Webbook

rinpol	1721.00	NIST Webbook
rinpol	1681.00	NIST Webbook
rinpol	1670.00	NIST Webbook
rinpol	1711.00	NIST Webbook
rinpol	1718.00	NIST Webbook
rinpol	1707.00	NIST Webbook
rinpol	1728.00	NIST Webbook
rinpol	1679.00	NIST Webbook
rinpol	1720.00	NIST Webbook
rinpol	1721.00	NIST Webbook
rinpol	1708.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1721.00	NIST Webbook
rinpol	1730.00	NIST Webbook
rinpol	1721.00	NIST Webbook
rinpol	1715.00	NIST Webbook
rinpol	1677.00	NIST Webbook
rinpol	1675.00	NIST Webbook
rinpol	1675.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1724.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1730.00	NIST Webbook
rinpol	1720.00	NIST Webbook
rinpol	1711.00	NIST Webbook
rinpol	1707.00	NIST Webbook
rinpol	1730.00	NIST Webbook
rinpol	1730.00	NIST Webbook
rinpol	1675.00	NIST Webbook
rinpol	1702.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1708.00	NIST Webbook
rinpol	1675.00	NIST Webbook
ripol	2466.00	NIST Webbook
ripol	2466.00	NIST Webbook
ripol	2420.00	NIST Webbook
ripol	2458.00	NIST Webbook
ripol	2386.00	NIST Webbook
ripol	2395.00	NIST Webbook
ripol	2458.00	NIST Webbook
ripol	2420.00	NIST Webbook
ripol	2423.00	NIST Webbook
ripol	2455.00	NIST Webbook

ripol	2400.00		NIST Webbook
ripol	2416.00		NIST Webbook
ripol	2470.00		NIST Webbook
ripol	2462.00		NIST Webbook
ripol	2455.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2406.00		NIST Webbook
ripol	2445.00		NIST Webbook
ripol	2426.00		NIST Webbook
ripol	2426.00		NIST Webbook
tb	588.28	K	Joback Method
tc	793.47	K	Joback Method
tf	327.17	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.14	J/mol×K	759.27	Joback Method
cpg	471.58	J/mol×K	588.28	Joback Method
cpg	491.03	J/mol×K	622.48	Joback Method
cpg	509.50	J/mol×K	656.68	Joback Method
cpg	527.01	J/mol×K	690.88	Joback Method
cpg	543.56	J/mol×K	725.07	Joback Method
cpg	573.78	J/mol×K	793.47	Joback Method
hvapt	84.60	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	399.20	K	0.10	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=C713951&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