«delta»-Nonalactone

Other names:	.delta.-nonanolactone
	2H-Pyran-2-one, 6-butyltetrahydro-
	2H-Pyran-2-one, tetrahydro-6-butyl
	5-Nonanolide
	6-butyltetrahydro-2H-pyran-2-one
	Nonan-1,5-olide
	«delta»-Butylvalerolactone
	«delta»-Nonanolide
	«delta»-nonanolactone
	Â«deltaÂ»-Butylvalerolactone
	Â«deltaÂ»-Nonanolide
	Â«deltaÂ»-nonanolactone
Inchi:	InChI=1S/C9H16O2/c1-2-3-5-8-6-4-7-9(10)11-8/h8H,2-7H2,1H3
InchiKey:	PXRBWNLUQYZAAX-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	156.22
CAS:	3301-94-8

Physical Properties

Property code	Value	Unit	Source
gf	-159.36	kJ/mol	Joback Method
hf	-444.47	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	70.70 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.272		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2023.00		NIST Webbook
tb	519.64	K	Joback Method
tc	734.94	K	Joback Method
tf	293.36	K	Joback Method

vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.40	J/mol×K	734.94	Joback Method
cpg	402.11	J/mol×K	699.06	Joback Method
cpg	387.99	J/mol×K	663.18	Joback Method
cpg	373.04	J/mol×K	627.29	Joback Method
cpg	357.27	J/mol×K	591.41	Joback Method
cpg	340.68	J/mol×K	555.52	Joback Method
cpg	323.28	J/mol×K	519.64	Joback Method
hvapt	71.10	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography
pvap	0.01	kPa	328.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	333.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	7.97e-03	kPa	323.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.03	kPa	343.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.05	kPa	348.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	5.09e-03	kPa	318.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	3.42e-03	kPa	313.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	2.14e-03	kPa	308.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	1.41e-03	kPa	303.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	8.60e-04	kPa	298.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	5.40e-04	kPa	293.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	338.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones

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=C3301948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of d-lactones:	https://www.doi.org/10.1016/j.jct.2006.06.010

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
pvap:	Vapor 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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