

2H-Pyran-2-one, tetrahydro-6-nonyl-

Other names:	«delta»-Nonyl-«delta»-valeralactone «delta»-Tetradecalactone «delta»-tetradecalactone tetrahydro-6-nonyl-2H-pyran-2-one
Inchi:	InChI=1S/C14H26O2/c1-2-3-4-5-6-7-8-10-13-11-9-12-14(15)16-13/h13H,2-12H2,1H3
InchiKey:	SKQYTJLYRIFFCO-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	226.35
CAS:	2721-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-117.26	kJ/mol	Joback Method
hf	-547.67	kJ/mol	Joback Method
hfus	31.34	kJ/mol	Joback Method
hvap	55.94	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.223		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
ripol	1938.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2675.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2675.00		NIST Webbook
tb	634.04	K	Joback Method
tc	833.46	K	Joback Method
tf	349.71	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.36	J/mol×K	634.04	Joback Method
cpg	598.62	J/mol×K	667.28	Joback Method
cpg	617.84	J/mol×K	700.51	Joback Method
cpg	636.02	J/mol×K	733.75	Joback Method
cpg	653.17	J/mol×K	766.99	Joback Method
cpg	669.30	J/mol×K	800.22	Joback Method
cpg	684.42	J/mol×K	833.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C2721224&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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