2-Oxepanone, 7-hexyl-

Other names:	«epsilon»-Dodecalactone
	7-Hexyl-2-oxepanone
	6-Hexylhexan-6-olide
	7-hexyloxepan-2-one
Inchi:	InChI=1S/C12H22O2/c1-2-3-4-5-8-11-9-6-7-10-12(13)14-11/h11H,2-10H2,1H3
InchiKey:	FRTMRFCNTDDSOB-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CCCCCCC1CCCCC(=O)O1
Mol. weight [g/mol]:	198.30
CAS:	16429-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-146.20	kJ/mol	Joback Method
hf	-512.55	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	51.66	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.443		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
ripol	2264.00		NIST Webbook
ripol	2264.00		NIST Webbook
tb	592.55	K	Joback Method
tc	804.62	K	Joback Method
tf	323.65	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.32	J/mol×K	592.55	Joback Method
cpg	493.76	J/mol×K	627.90	Joback Method
cpg	513.14	J/mol×K	663.24	Joback Method

cpg	531.45	J/mol×K	698.59	Joback Method
cpg	548.69	J/mol×K	733.93	Joback Method
cpg	564.86	J/mol×K	769.28	Joback Method
cpg	579.96	J/mol×K	804.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16429213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume