2-Oxecanone, 10-methyl-, (.+/-.)-

Other names: (.+/-.)-Decan-9-olide
(.+/-.)-Phoracantholide I
9-Decanolide
10-Methyl-2-oxecanone
Inchi: InChI=1S/C10H18O2/c1-9-7-5-3-2-4-6-8-10(11)12-9/h9H,2-8H2,1H3
InchiKey: SAMJSVOFANTIOD-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC1CCCCCCCC(=O)O1
Mol. weight [g/mol]: 170.25
CAS: 65371-24-6

Physical Properties

Property code	Value	Unit	Source
gf	-199.34	kJ/mol	Joback Method
hf	-489.75	kJ/mol	Joback Method
hfus	12.58	kJ/mol	Joback Method
hvap	47.73	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1308.00		NIST Webbook
tb	559.60	K	Joback Method
tc	804.37	K	Joback Method
tf	290.55	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.10	J/mol×K	559.60	Joback Method
cpg	397.87	J/mol×K	600.39	Joback Method
cpg	419.38	J/mol×K	641.19	Joback Method
cpg	439.56	J/mol×K	681.98	Joback Method

cpg	458.38	J/mol×K	722.78	Joback Method
cpg	475.78	J/mol×K	763.57	Joback Method
cpg	491.70	J/mol×K	804.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65371246&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume