3,7-Dimethyl-oct-6-en-4-olide

Inchi: InChI=1S/C10H16O2/c1-7(2)4-5-9-8(3)6-10(11)12-9/h4-5,7-9H,6H2,1-3H3/b5-4+
InchiKey: MLFXHMZNLOGDGV-SNAWJCMRSA-N
Formula: C10H16O2
SMILES: CC(C)C=CC1OC(=O)CC1C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-68.77	kJ/mol	Joback Method
hf	-367.35	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.150		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
ripol	2058.00		NIST Webbook
ripol	2058.00		NIST Webbook
tb	537.30	K	Joback Method
tc	755.78	K	Joback Method
tf	283.83	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.30	J/mol×K	537.30	Joback Method
cpg	371.01	J/mol×K	573.71	Joback Method
cpg	387.82	J/mol×K	610.13	Joback Method
cpg	403.72	J/mol×K	646.54	Joback Method
cpg	418.73	J/mol×K	682.95	Joback Method
cpg	432.87	J/mol×K	719.37	Joback Method
cpg	446.14	J/mol×K	755.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326180&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