2,6,6-trimethyl-3-oxo-1-cyclohexene-1-carboxalde

Other names: 2,6,6-Trimethyl-3-oxocyclohex-1-ene-1-carbaldehyde
Oxo-«beta»-cyclocitral
Inchi: InChI=1S/C10H14O2/c1-7-8(6-11)10(2,3)5-4-9(7)12/h6H,4-5H2,1-3H3
InchiKey: FRKQOTHZPTXCJI-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC1=C(C=O)C(C)(C)CCC1=O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-159.13	kJ/mol	Joback Method
hf	-368.61	kJ/mol	Joback Method
hfus	9.44	kJ/mol	Joback Method
hvap	49.72	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.891		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1304.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	573.59	K	Joback Method
tc	803.68	K	Joback Method
tf	369.76	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.38	J/mol×K	573.59	Joback Method
cpg	356.53	J/mol×K	611.94	Joback Method
cpg	370.89	J/mol×K	650.29	Joback Method
cpg	384.55	J/mol×K	688.64	Joback Method

cpg	397.59	J/mol×K	726.99	Joback Method
cpg	410.10	J/mol×K	765.33	Joback Method
cpg	422.17	J/mol×K	803.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407006&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