Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester

Other names:	Methyl (3-oxo-2-pentylcyclopentyl)acetate
	Hedione
	Kharismal
	Methyl (2-pentyl-3-oxocyclopentyl)acetate
	Methyl dihydrojasmonate
	Methyl hydrojasmonate
	methyl 3-oxo-2-pentylcyclopentaneacetate
Inchi:	InChI=1S/C13H22O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h10-11H,3-9H2,1-2H3
InchiKey:	KVWWIYGFBYDJQC-UHFFFAOYSA-N
Formula:	C13H22O3
SMILES:	CCCCCC1C(=O)CCC1CC(=O)OC
Mol. weight [g/mol]:	226.31
CAS:	24851-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-269.09	kJ/mol	Joback Method
hf	-654.01	kJ/mol	Joback Method
hfus	26.73	kJ/mol	Joback Method
hvap	57.88	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.725		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2241.00		NIST Webbook

tb	651.56	K	Joback Method
tc	854.07	K	Joback Method
tf	383.31	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.32	J/mol×K	651.56	Joback Method
cpg	562.70	J/mol×K	685.31	Joback Method
cpg	580.11	J/mol×K	719.06	Joback Method
cpg	596.55	J/mol×K	752.81	Joback Method
cpg	612.00	J/mol×K	786.57	Joback Method
cpg	626.46	J/mol×K	820.32	Joback Method
cpg	639.93	J/mol×K	854.07	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24851987&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume