4-(1,2-Dimethyl-cyclopent-2-enyl)-butan-2-one

Inchi: InChI=1S/C11H18O/c1-9-5-4-7-11(9,3)8-6-10(2)12/h5H,4,6-8H2,1-3H3
InchiKey: FJXCDFSRZLXRTG-UHFFFAOYSA-N
Formula: C11H18O
SMILES: CC(=O)CCC1(C)CCC=C1C
Mol. weight [g/mol]: 166.26
CAS: 75698-06-5

Physical Properties

Property code	Value	Unit	Source
gf	-35.79	kJ/mol	Joback Method
hf	-260.92	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	46.89	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.102		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1240.00		NIST Webbook
rinpol	1265.00		NIST Webbook
tb	524.61	K	Joback Method
tc	732.83	K	Joback Method
tf	311.74	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.07	J/mol×K	524.61	Joback Method
cpg	374.53	J/mol×K	559.31	Joback Method
cpg	389.98	J/mol×K	594.02	Joback Method
cpg	404.53	J/mol×K	628.72	Joback Method
cpg	418.28	J/mol×K	663.42	Joback Method
cpg	431.34	J/mol×K	698.12	Joback Method
cpg	443.83	J/mol×K	732.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75698065&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