4,4-Dimethyl-2-cyclopenten-1-one

Inchi: InChI=1S/C7H10O/c1-7(2)4-3-6(8)5-7/h3-4H,5H2,1-2H3
InchiKey: YVFVCSCZJJGBAK-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC1(C)C=CC(=O)C1
Mol. weight [g/mol]: 110.15
CAS: 22748-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-53.51	kJ/mol	Joback Method
hf	-192.01	kJ/mol	Joback Method
hfus	2.25	kJ/mol	Joback Method
hvap	34.82	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.542		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
ripol	1511.00		NIST Webbook
tb	431.20	K	NIST Webbook
tc	669.24	K	Joback Method
tf	272.43	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.44	J/mol×K	442.06	Joback Method
cpg	205.04	J/mol×K	479.92	Joback Method
cpg	217.69	J/mol×K	517.79	Joback Method
cpg	229.51	J/mol×K	555.65	Joback Method
cpg	240.59	J/mol×K	593.51	Joback Method
cpg	251.02	J/mol×K	631.37	Joback Method
cpg	260.90	J/mol×K	669.24	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22748169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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