4-[2,2-Dimethyl-3-(5-methylcyclopenta-1,4-dien-1-
2-one

Inchi: InChI=1S/C15H24O/c1-10-6-5-7-12(10)14-13(15(14,3)4)9-8-11(2)16/h6,12-14H,5,7-9H2,

InchiKey: UQXZKPUZCLFORX-KFTPUPIBSA-N

Formula: C15H24O

SMILES: CC(=O)CCC1C(C2CCC=C2C)C1(C)C

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	43.22	kJ/mol	Joback Method
hf	-311.36	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1586.00		NIST Webbook
tb	613.53	K	Joback Method
tc	822.96	K	Joback Method
tf	366.28	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.29	J/mol×K	613.53	Joback Method
cpg	567.51	J/mol×K	648.43	Joback Method
cpg	586.62	J/mol×K	683.34	Joback Method
cpg	604.75	J/mol×K	718.24	Joback Method
cpg	622.04	J/mol×K	753.15	Joback Method
cpg	638.61	J/mol×K	788.05	Joback Method
cpg	654.60	J/mol×K	822.96	Joback Method

Sources

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=R407808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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