2,4-Cycloheptadien-1-one, 2,6,6-trimethyl-

Other names:	Eucarvone
	2,6,6-Trimethyl-2,4-cycloheptadien-1-one
Inchi:	InChI=1S/C10H14O/c1-8-5-4-6-10(2,3)7-9(8)11/h4-6H,7H2,1-3H3
InchiKey:	QNGQIURXCUHNAT-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC1=CC=CC(C)(C)CC1=O
Mol. weight [g/mol]:	150.22
CAS:	503-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-32.12	kJ/mol	Joback Method
hf	-219.94	kJ/mol	Joback Method
hfus	6.66	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
ie	9.62	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1222.70		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1222.70		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1248.00		NIST Webbook
tb	523.38	K	Joback Method
tc	760.57	K	Joback Method
tf	312.48	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.42	J/mol×K	523.38	Joback Method
cpg	320.39	J/mol×K	562.91	Joback Method
cpg	336.37	J/mol×K	602.44	Joback Method
cpg	351.45	J/mol×K	641.98	Joback Method
cpg	365.72	J/mol×K	681.51	Joback Method
cpg	379.28	J/mol×K	721.04	Joback Method
cpg	392.23	J/mol×K	760.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C503935&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
ie: Ionization energy
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