2,5,6,6-Tetramethylcyclohexe-2-en-1-one

Inchi: InChI=1S/C10H16O/c1-7-5-6-8(2)10(3,4)9(7)11/h5,8H,6H2,1-4H3
InchiKey: KXRGNMKZVAJQJO-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CCC(C)C(C)(C)C1=O
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-57.69	kJ/mol	Joback Method
hf	-291.90	kJ/mol	Joback Method
hfus	8.61	kJ/mol	Joback Method
hvap	42.02	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
ripol	1405.00		NIST Webbook
ripol	1405.00		NIST Webbook
tb	515.28	K	Joback Method
tc	741.26	K	Joback Method
tf	311.00	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.92	J/mol×K	515.28	Joback Method
cpg	339.56	J/mol×K	552.94	Joback Method
cpg	356.26	J/mol×K	590.61	Joback Method
cpg	372.09	J/mol×K	628.27	Joback Method
cpg	387.13	J/mol×K	665.93	Joback Method
cpg	401.47	J/mol×K	703.59	Joback Method
cpg	415.19	J/mol×K	741.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519045&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume