2-Cyclohexen-1-one, 3-methyl-6-(1-methylethenyl)-

Other names: p-Mentha-1,8-dien-3-one
Isopiperitenon
Isopiperitenone

Inchi: InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)6-10(9)11/h6,9H,1,4-5H2,2-3H3

InchiKey: SEZLYIWMVRUIKT-UHFFFAOYSA-N

Formula: C10H14O

SMILES: C=C(C)C1CCC(C)=CC1=O

Mol. weight [g/mol]: 150.22

CAS: 529-01-1

Physical Properties

Property code	Value	Unit	Source
gf	34.80	kJ/mol	Joback Method
hf	-171.16	kJ/mol	Joback Method
hfus	11.24	kJ/mol	Joback Method
hvap	42.89	kJ/mol	Joback Method
ie	9.53	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1266.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1832.00		NIST Webbook

ripol	1865.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1865.00		NIST Webbook
tb	516.27	K	Joback Method
tc	742.23	K	Joback Method
tf	275.62	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.34	J/mol×K	516.27	Joback Method
cpg	319.31	J/mol×K	553.93	Joback Method
cpg	335.43	J/mol×K	591.59	Joback Method
cpg	350.72	J/mol×K	629.25	Joback Method
cpg	365.16	J/mol×K	666.91	Joback Method
cpg	378.76	J/mol×K	704.57	Joback Method
cpg	391.51	J/mol×K	742.23	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=C529011&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume