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

Other names: p-Mentha-1,4(8)-dien-3-one
Piperitenone
Pulespenone
3-Terpinolenone
3-methyl-6-(1-methylethylidene)cyclohex-2-en-1-one

Inchi: InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)6-10(9)11/h6H,4-5H2,1-3H3

InchiKey: HKZQJZIFODOLFR-UHFFFAOYSA-N

Formula: C10H14O

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

Mol. weight [g/mol]: 150.22

CAS: 491-09-8

Physical Properties

Property code	Value	Unit	Source
gf	0.13	kJ/mol	Joback Method
hf	-200.22	kJ/mol	Joback Method
hfus	11.78	kJ/mol	Joback Method
hvap	44.66	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.632		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	1304.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1315.00		NIST Webbook

rinpol	1316.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1340.00	NIST Webbook
rinpol	1329.00	NIST Webbook
rinpol	1297.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1311.00	NIST Webbook
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rinpol	1317.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1336.00	NIST Webbook
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rinpol	1320.00	NIST Webbook
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rinpol	1315.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1347.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1310.00	NIST Webbook
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rinpol	1343.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1329.00	NIST Webbook
rinpol	1348.00	NIST Webbook

ripol	1949.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	530.90	K	Joback Method
tc	759.57	K	Joback Method
tf	291.98	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.20	J/mol×K	530.90	Joback Method
cpg	318.22	J/mol×K	569.01	Joback Method
cpg	333.43	J/mol×K	607.12	Joback Method
cpg	347.84	J/mol×K	645.23	Joback Method
cpg	361.44	J/mol×K	683.34	Joback Method
cpg	374.25	J/mol×K	721.46	Joback Method
cpg	386.27	J/mol×K	759.57	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=C491098&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume