2-Cyclohexen-1-one, 4-(1-methylethyl)-

Other names:	4-Isopropylcyclohex-2-enone
	Crypton
	Cryptone
	Cryptone, L-
	2-Cyclohexen-1-one, 4-isopropyl-
	4-(1-Methylethyl)-2-cyclohexen-1-one
	4-Isopropyl-2-cyclohexenone
	4-Isopropyl-2-cyclohexen-1-one
	Kryptone
	NSC 22060
	2-Cyclohexenone, 4-isopropyl
	Criptone
	4-isopropylcyclohex-2-en-1-one
Inchi:	InChI=1S/C9H14O/c1-7(2)8-3-5-9(10)6-4-8/h3,5,7-8H,4,6H2,1-2H3
InchiKey:	AANMVENRNJYEMK-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(C)C1C=CC(=O)CC1
Mol. weight [g/mol]:	138.21
CAS:	500-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-45.72	kJ/mol	Joback Method
hf	-259.97	kJ/mol	Joback Method
hfus	8.11	kJ/mol	Joback Method
hvap	40.21	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1160.00		NIST Webbook

rinpol	1159.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1181.00	NIST Webbook
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ripol	1658.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	491.41	K	Joback Method
tc	715.76	K	Joback Method
tf	252.55	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	275.08	J/mol×K	491.41	Joback Method
cpg	292.29	J/mol×K	528.80	Joback Method
cpg	308.67	J/mol×K	566.19	Joback Method
cpg	324.21	J/mol×K	603.58	Joback Method
cpg	338.91	J/mol×K	640.98	Joback Method
cpg	352.76	J/mol×K	678.37	Joback Method
cpg	365.78	J/mol×K	715.76	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=C500027&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