Cyclohexanone, 5-methyl-2-(1-methylethyl)-, cis-

Other names: p-Menthan-3-one, cis-
cis-p-Menthan-3-one
Isomenthone
p-Menthan-3-one, (Z)-
Cyclohexanone, 5-methyl-2-(1-methylethyl)-, (Z)-
2-Isopropyl-5-methyl-cyclohexanone, cis
5-Methyl-2-(1-methylethyl)cyclohexanone, (Z)-
«alpha»-Isomenthone
cis-5-Methyl-2-(1-methylethyl)-cyclohexanone
Isomenthon
cis-Menthone
cis-p-Menthone
(2R,5R)-2-isopropyl-5-methylcyclohexanone, rel-
Cyclohexanone, 5-methyl-2-(1-methylethyl)-, (2R,5R)-rel-
dl-Isomenthone

Inchi: InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-9H,4-6H2,1-3H3/t8-,9-/m1/s1

InchiKey: NFLGAXVYCFJBMK-RKDXNWHRSA-N

Formula: C10H18O

SMILES: CC1CCC(C(C)C)C(=O)C1

Mol. weight [g/mol]: 154.25

CAS: 491-07-6

Physical Properties

Property code	Value	Unit	Source
gf	-74.97	kJ/mol	Joback Method
hf	-358.73	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.648		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1153.00		NIST Webbook

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ripol	1502.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1528.00		NIST Webbook
tb	510.46	K	Joback Method

tc	728.68	K	Joback Method
tf	258.82	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.98	J/mol×K	510.46	Joback Method
cpg	358.78	J/mol×K	546.83	Joback Method
cpg	377.66	J/mol×K	583.20	Joback Method
cpg	395.62	J/mol×K	619.57	Joback Method
cpg	412.65	J/mol×K	655.94	Joback Method
cpg	428.75	J/mol×K	692.31	Joback Method
cpg	443.91	J/mol×K	728.68	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=C491076&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

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