4-ISOPROPYLCYCLOHEXANONE

Other names:	4-isopropylcyclohexan-1-one
	Cyclohexanone, 4-(1-methylethyl)-
	Cyclohexanone, 4-isopropyl-
Inchi:	InChI=1S/C9H16O/c1-7(2)8-3-5-9(10)6-4-8/h7-8H,3-6H2,1-2H3
InchiKey:	FPKISACHVIIMRA-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CC(C)C1CCC(=O)CC1
Mol. weight [g/mol]:	140.23
CAS:	5432-85-9

Physical Properties

Property code	Value	Unit	Source
af	0.3719		Cheméo Relay (1.0)
hf	-278.79	kJ/mol	Cheméo Relay (1.0)
hfus	6.89	kJ/mol	Joback Method
hvap	53.07	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1182.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	478.77	K	Cheméo Relay (1.0)
tc	685.00	K	Cheméo Relay (1.0)
tf	246.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.68	J/mol×K	492.25	Joback Method
cpg	310.17	J/mol×K	529.26	Joback Method
cpg	327.79	J/mol×K	566.26	Joback Method
cpg	344.53	J/mol×K	603.27	Joback Method

cpg	360.40	J/mol×K	640.28	Joback Method
cpg	375.38	J/mol×K	677.29	Joback Method
cpg	389.49	J/mol×K	714.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.70	K	13.30	NIST Webbook
tbrp	368.00 ± 1.00	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61205e+01
Coeff. B	-4.52411e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	362.32
Temperature range (K), max.	495.13

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5432859&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point