

Isophorone

Other names:	1,1,3-Trimethyl-3-cyclohexene-5-one 2-Cyclohexen-1-one, 3,5,5-trimethyl- 2-cyclohexene-1-one, 3,5,5-trimethyl- 3,3,5-Trimethyl-2-cyclohexen-1-one 3,5,5-Trimethyl-2-cyclohexen-1-on 3,5,5-Trimethyl-2-cyclohexen-1-one 3,5,5-Trimethyl-2-cyclohexene-1-one 3,5,5-Trimethyl-2-cyclohexenone 3,5,5-Trimethylcyclohex-2-enone 3,5,5-Trimethylcyclohexen-2-one-1 3,5,5-Trimetil-2-cicloesen-1-one 3,5,5-trimethylcyclohex-2-en-1-one Isoacetophorone Isoforon Isoforone Isophoron Izoforon NCI-C55618 NSC 403657 «alpha»-Isophoron «alpha»-Isophorone Â«alphaÂ»-Isophoron Â«alphaÂ»-Isophorone
Inchi:	InChI=1S/C9H14O/c1-7-4-8(10)6-9(2,3)5-7/h4H,5-6H2,1-3H3
InchiKey:	HJOVHMDZYOCNQW-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1=CC(=O)CC(C)(C)C1
Mol. weight [g/mol]:	138.21
CAS:	78-59-1

Physical Properties

Property code	Value	Unit	Source
affp	893.50	kJ/mol	NIST Webbook
basg	861.60	kJ/mol	NIST Webbook
chl	-5265.10	kJ/mol	NIST Webbook
gf	-58.40	kJ/mol	Joback Method

hf	-250.92	kJ/mol	Joback Method
hfus	4.95	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
ie	9.07	eV	NIST Webbook
log10ws	-1.06		Aqueous Solubility Prediction Method
log10ws	-1.06		Estimated Solubility Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1067.00		NIST Webbook
rinpol	186.60		NIST Webbook
rinpol	187.34		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1080.70		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1128.05		NIST Webbook

rinpol	1080.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1123.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	187.71	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1120.90	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1119.00	NIST Webbook
rinpol	1116.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1119.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1126.00	NIST Webbook
ripol	1577.00	NIST Webbook

ripol	1569.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1544.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1543.00		NIST Webbook
tb	488.45	K	NIST Webbook
tb	486.70	K	NIST Webbook
tc	727.23	K	Joback Method
tf	265.05	K	NIST Webbook
tf	265.12	K	Aqueous Solubility Prediction Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.69	J/mol×K	497.07	Joback Method

cpg	291.98	J/mol×K	535.43	Joback Method
cpg	307.32	J/mol×K	573.79	Joback Method
cpg	321.80	J/mol×K	612.15	Joback Method
cpg	335.52	J/mol×K	650.51	Joback Method
cpg	348.57	J/mol×K	688.87	Joback Method
cpg	361.03	J/mol×K	727.23	Joback Method
hvapt	48.60	kJ/mol	400.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Measurement and Correlation of Ternary (Liquid + Liquid) Equilibria for Separation of Phase Equilibrium of a Quaternary System at 500 kPa:	https://www.doi.org/10.1021/acs.jced.7b00787
Joback Method:	https://www.doi.org/10.1021/acs.jced.8b00273
Aqueous Solubility Prediction Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78591&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
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

Latest version available from:

<https://www.chemeo.com/cid/61-403-6/Isophorone.pdf>

Generated by Cheméo on 2025-12-05 14:46:09.254562207 +0000 UTC m=+4694166.784602861.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.