2,6,6-Trimethyl-2-cyclohexene-1,4-dione

Other names:	2-Cyclohexene-1,4-dione, 2,6,6-trimethyl-
	4-Oxoisophorone
	2,2,6-trimethylcyclohex-2-en-1,4-dione
	2,6,6-Trimethyl-2-cyclohexen-1,4-dione
	2,6,6-trimethylcyclohex-2-ene-1,4-dione
	2-Cyclohexen-1,4-dione, 2,6,6-trimethyl
	3,5,5-trimethyl-2-cyclohexene-1,4-dione
	3,5,5-Trimethylcyclohex-2-en-1,4-dione
	3,5,5-trimethylcyclohex-2-ene-1,4-dione
	4-Ketoisophorone
	Ketoisophorone
	Oxoisophorone
	Oxopholone
	4-Oxo-«alpha»-isophorone
	2,6,6-Trimethylcyclohex-2-en-1,4-dione
	2,2,6-Trimethylcyclohex-2-en-1,4-dione (4-oxoisophorone)
	2,6,6-Trimethy-2-cyclohexene-1,4-dione (4-oxoisophorone)
	Oxophorone
	Cyclohexen-1,4-dione, 2,6,6-trimethyl
	2,2,6-trimethyl-2-cyclohexene-1,4-dione (cetoisophorone)
Inchi:	InChI=1S/C9H12O2/c1-6-4-7(10)5-9(2,3)8(6)11/h4H,5H2,1-3H3
InchiKey:	AYJXHIDNNLJQDT-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC1=CC(=O)CC(C)(C)C1=O
Mol. weight [g/mol]:	152.19
CAS:	1125-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-180.99	kJ/mol	Joback Method
hf	-388.62	kJ/mol	Joback Method
hfus	4.46	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.501		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method

rinpol	1142.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1166.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1142.10	NIST Webbook
rinpol	1159.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1105.10	NIST Webbook
rinpol	1105.10	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1105.10	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1159.00	NIST Webbook
rinpol	1117.00	NIST Webbook
ripol	1671.00	NIST Webbook
ripol	1672.00	NIST Webbook
ripol	1668.00	NIST Webbook
ripol	1655.00	NIST Webbook
ripol	1706.00	NIST Webbook
ripol	1676.00	NIST Webbook

ripol	1708.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1693.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	564.89	K	Joback Method
tc	810.92	K	Joback Method
tf	372.19	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.69	J/mol×K	564.89	Joback Method
cpg	318.39	J/mol×K	605.89	Joback Method
cpg	333.34	J/mol×K	646.90	Joback Method
cpg	347.58	J/mol×K	687.90	Joback Method
cpg	361.20	J/mol×K	728.91	Joback Method
cpg	374.24	J/mol×K	769.91	Joback Method
cpg	386.78	J/mol×K	810.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.20	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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