1-Propen-1-one, 2-methyl-

Other names:	(CH3)2C=C=O
	1,1-Dimethylketene
	2-methyl-1-propen-1-one
	Ketene, dimethyl-
Inchi:	InChI=1S/C4H6O/c1-4(2)3-5/h1-2H3
InchiKey:	VDOKWPVSGXHSNP-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	CC(C)=C=O
Mol. weight [g/mol]:	70.09
CAS:	598-26-5

Physical Properties

Property code	Value	Unit	Source
hfus	12.34	kJ/mol	Joback Method
ie	8.38	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
logp	0.784		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
rinpol	484.00		NIST Webbook
rinpol	484.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1215.00		NIST Webbook
tb	310.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.99	J/mol×K	284.95	Joback Method
cpg	97.10	J/mol×K	312.18	Joback Method
cpg	102.92	J/mol×K	339.41	Joback Method
cpg	108.47	J/mol×K	366.64	Joback Method
cpg	113.76	J/mol×K	393.87	Joback Method
cpg	118.80	J/mol×K	421.10	Joback Method

cpg	123.59	J/mol×K	448.33	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64479e+01
Coeff. B	-3.63072e+03
Coeff. C	-4.27740e+01
Temperature range (K), min.	267.44
Temperature range (K), max.	389.81

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=C598265&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

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pvap: Vapor pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature