1,2-Propadiene-1,3-dione

Other names:	Carbon suboxide
	Carbon oxide (C3O2)
	C3O2
Inchi:	InChI=1S/C3O2/c4-2-1-3-5
InchiKey:	GNEVIACKFGQMHB-UHFFFAOYSA-N
Formula:	C3O2
SMILES:	O=C=C=C=O
Mol. weight [g/mol]:	68.03
CAS:	504-64-3

Physical Properties

Property code	Value	Unit	Source
chl	-1059.10	kJ/mol	NIST Webbook
ea	0.85 ± 0.15	eV	NIST Webbook
gf	-37.68	kJ/mol	Joback Method
hf	-97.80 ± 1.80	kJ/mol	NIST Webbook
hfl	-121.50 ± 1.00	kJ/mol	NIST Webbook
hfus	20.53	kJ/mol	Joback Method
hvap	35.10	kJ/mol	Joback Method
ie	10.60	eV	NIST Webbook
ie	10.60 ± 0.03	eV	NIST Webbook
ie	10.61	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
log10ws	-8.69		Crippen Method
logp	-0.639		Crippen Method
mcvol	47.670	ml/mol	McGowan Method
pc	9920.48	kPa	Joback Method
tb	255.45	K	Joback Method
tc	413.48	K	Joback Method
tf	180.00	K	Joback Method
vc	0.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	75.13	J/mol×K	255.45	Joback Method
cpg	76.52	J/mol×K	281.79	Joback Method
cpg	77.84	J/mol×K	308.13	Joback Method
cpg	79.11	J/mol×K	334.47	Joback Method
cpg	80.31	J/mol×K	360.81	Joback Method
cpg	81.46	J/mol×K	387.14	Joback Method
cpg	82.55	J/mol×K	413.48	Joback Method
hvapt	26.20	kJ/mol	205.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C504643&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume