Propanal, 2,2-dimethyl-

Other names:	2,2-Dimethylpropanal
	2,2-Dimethylpropionaldehyde
	NSC 22043
	Neopentanal
	Pivalaldehyde
	Pivaldehyde
	Pivalic aldehyde
	Trimethylacetaldehyde
	tert-C4H9CHO
	tert-Valeraldehyde
	«alpha»,«alpha»-Dimethylpropionaldehyde
	Â«alphaÂ»,Â«alphaÂ»-Dimethylpropionaldehyde
Inchi:	InChI=1S/C5H10O/c1-5(2,3)4-6/h4H,1-3H3
InchiKey:	FJJYHTVHBVXEEQ-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC(C)(C)C=O
Mol. weight [g/mol]:	86.13
CAS:	630-19-3

Physical Properties

Property code	Value	Unit	Source
ea	5.21e-04	eV	NIST Webbook
gf	-105.46	kJ/mol	Joback Method
hf	-240.86	kJ/mol	Joback Method
hfus	3.58	kJ/mol	Joback Method
hvap	32.15	kJ/mol	Joback Method
ie	9.51	eV	NIST Webbook
ie	9.50 ± 0.01	eV	NIST Webbook
ie	9.51 ± 0.01	eV	NIST Webbook
ie	9.51 ± 0.01	eV	NIST Webbook
log10ws	-0.95		Crippen Method
logp	1.231		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	582.00		NIST Webbook
rinpol	586.08		NIST Webbook
rinpol	580.50		NIST Webbook

rinpol	581.71		NIST Webbook
rinpol	583.28		NIST Webbook
rinpol	584.49		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	583.00		NIST Webbook
ripol	831.10		NIST Webbook
ripol	826.70		NIST Webbook
ripol	809.00		NIST Webbook
ripol	807.00		NIST Webbook
ripol	835.60		NIST Webbook
ripol	822.60		NIST Webbook
ripol	809.00		NIST Webbook
sl	262.05	J/mol×K	NIST Webbook
tb	359.23	K	Joback Method
tc	544.03	K	Joback Method
tf	276.00 ± 3.00	K	NIST Webbook
tf	279.00 ± 2.00	K	NIST Webbook
tf	277.00 ± 0.60	K	NIST Webbook
tf	279.00 ± 3.00	K	NIST Webbook
tf	276.00 ± 4.00	K	NIST Webbook
tt	272.10 ± 0.20	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.13	J/mol×K	544.03	Joback Method
cpg	155.34	J/mol×K	390.03	Joback Method
cpg	164.66	J/mol×K	420.83	Joback Method
cpg	173.48	J/mol×K	451.63	Joback Method
cpg	181.81	J/mol×K	482.43	Joback Method
cpg	189.69	J/mol×K	513.23	Joback Method
cpg	145.50	J/mol×K	359.23	Joback Method
cpl	192.80	J/mol×K	298.43	NIST Webbook
cpl	185.58	J/mol×K	298.15	NIST Webbook
dvisc	0.0003603	Pa×s	359.23	Joback Method

dvisc	0.0010168	Pa×s	274.88	Joback Method
dvisc	0.0016821	Pa×s	246.76	Joback Method
dvisc	0.0071887	Pa×s	190.53	Joback Method
dvisc	0.0031673	Pa×s	218.65	Joback Method
dvisc	0.0004801	Pa×s	331.11	Joback Method
dvisc	0.0006748	Pa×s	303.00	Joback Method
hfust	4.81	kJ/mol	183.90	NIST Webbook
hfust	2.52	kJ/mol	272.10	NIST Webbook
hfust	0.50	kJ/mol	158.50	NIST Webbook
hfust	2.52	kJ/mol	272.10	NIST Webbook
hvapt	34.20	kJ/mol	322.00	NIST Webbook
sfust	9.26	J/mol×K	272.10	NIST Webbook
sfust	26.15	J/mol×K	183.90	NIST Webbook
sfust	3.15	J/mol×K	158.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.20	K	97.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40634e+01
Coeff. B	-2.73766e+03
Coeff. C	-5.81500e+01
Temperature range (K), min.	256.88
Temperature range (K), max.	370.96

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630193&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume