Propanoic acid, 2,2-dimethyl-

Other names:	2,2-Dimethylpropanoic acid
	2,2-Dimethylpropionic acid
	Acetic acid, trimethyl-
	DIMETHYLPROPIONIC ACID
	Kyselina 2,2-dimethylpropionova
	Kyselina pivalova
	NEOPENTANOIC ACID
	NSC 65449
	Neovaleric acid
	PIVALIC ACID
	Propionic acid, 2,2-dimethyl-
	TERT-PENTANOIC ACID
	Trimethylacetic acid
	Versatic 5
	tert-C4H9COOH
	«alpha»,«alpha»-Dimethylpropionic acid
	Â«alphaÂ»,Â«alphaÂ»-Dimethylpropionic acid
Inchi:	InChI=1S/C5H10O2/c1-5(2,3)4(6)7/h1-3H3,(H,6,7)
InchiKey:	IUGYQRQAERSCNH-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC(C)(C)C(=O)O
Mol. weight [g/mol]:	102.13
CAS:	75-98-9

Physical Properties

Property code	Value	Unit	Source
chs	-2832.10 ± 5.90	kJ/mol	NIST Webbook
gf	-271.68	kJ/mol	Joback Method
hf	-420.09	kJ/mol	Joback Method
hfs	-564.50 ± 5.90	kJ/mol	NIST Webbook
hfus	6.98	kJ/mol	Joback Method
hsub	73.20 ± 3.00	kJ/mol	NIST Webbook
hvap	48.85	kJ/mol	Joback Method
ie	10.08	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
log10ws	-0.77		Crippen Method
logp	1.117		Crippen Method

mcvol	88.750	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	864.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1527.00		NIST Webbook
tb	436.65 ± 3.00	K	NIST Webbook
tb	374.60 ± 2.00	K	NIST Webbook
tb	423.65 ± 5.00	K	NIST Webbook
tb	374.80 ± 2.00	K	NIST Webbook
tb	436.65 ± 2.00	K	NIST Webbook
tb	431.15 ± 5.00	K	NIST Webbook
tb	434.65 ± 3.00	K	NIST Webbook
tb	437.65 ± 1.00	K	NIST Webbook
tb	437.55 ± 0.50	K	NIST Webbook
tb	436.95 ± 1.00	K	NIST Webbook
tb	375.20 ± 2.00	K	NIST Webbook
tb	436.15 ± 3.00	K	NIST Webbook
tb	434.65 ± 4.00	K	NIST Webbook
tb	432.65 ± 4.00	K	NIST Webbook
tb	446.65 ± 5.00	K	NIST Webbook
tb	437.15 ± 1.50	K	NIST Webbook
tb	435.00 ± 3.00	K	NIST Webbook
tb	437.32 ± 0.50	K	NIST Webbook
tb	436.65 ± 2.00	K	NIST Webbook
tb	437.15 ± 1.50	K	NIST Webbook
tb	432.15 ± 3.00	K	NIST Webbook
tb	437.35 ± 1.00	K	NIST Webbook
tb	436.65 ± 3.00	K	NIST Webbook
tb	436.50 ± 0.50	K	NIST Webbook
tb	436.15 ± 2.00	K	NIST Webbook
tb	437.15 ± 2.00	K	NIST Webbook
tb	437.20	K	NIST Webbook
tb	436.65 ± 2.00	K	NIST Webbook
tb	436.90 ± 2.00	K	NIST Webbook
tb	436.15 ± 2.00	K	NIST Webbook
tb	436.00 ± 4.00	K	NIST Webbook
tb	436.15 ± 2.00	K	NIST Webbook

tc	639.96	K	Joback Method
tf	309.08 ± 0.01	K	NIST Webbook
tf	308.55 ± 0.50	K	NIST Webbook
tf	308.55 ± 0.25	K	NIST Webbook
tf	308.82 ± 0.20	K	NIST Webbook
tf	306.25 ± 1.50	K	NIST Webbook
tf	304.00 ± 2.00	K	NIST Webbook
tf	308.15 ± 1.50	K	NIST Webbook
tf	307.15 ± 1.00	K	NIST Webbook
tf	307.20 ± 4.00	K	NIST Webbook
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.55	J/mol×K	487.18	Joback Method
cpg	203.75	J/mol×K	517.73	Joback Method
cpg	211.50	J/mol×K	548.29	Joback Method
cpg	218.81	J/mol×K	578.85	Joback Method
cpg	225.71	J/mol×K	609.41	Joback Method
cpg	232.22	J/mol×K	639.96	Joback Method
cpg	186.87	J/mol×K	456.62	Joback Method
cps	192.20	J/mol×K	298.15	NIST Webbook
cps	178.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0002510	Pa×s	456.62	Joback Method
dvisc	0.0007550	Pa×s	390.84	Joback Method
dvisc	0.0015240	Pa×s	357.95	Joback Method
dvisc	0.0035460	Pa×s	325.06	Joback Method
dvisc	0.0099787	Pa×s	292.17	Joback Method
dvisc	0.0004171	Pa×s	423.73	Joback Method
dvisc	0.0365089	Pa×s	259.28	Joback Method
hfust	2.27	kJ/mol	309.10	NIST Webbook
hfust	2.30	kJ/mol	309.10	NIST Webbook
hsubt	62.30	kJ/mol	291.00	NIST Webbook
hvapt	47.00 ± 0.40	kJ/mol	408.00	NIST Webbook
hvapt	50.90 ± 0.20	kJ/mol	408.00	NIST Webbook
hvapt	57.60 ± 0.20	kJ/mol	408.00	NIST Webbook
hvapt	54.40 ± 0.20	kJ/mol	408.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38753e+01
Coeff. B	-2.97668e+03
Coeff. C	-1.19330e+02
Temperature range (K), min.	309.08
Temperature range (K), max.	466.92

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=937
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75989&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume