2,3-Pentanedione

Other names:	2,3-Pentadione
	2,3-Pentandione
	Acetylpropionyl
	CH3C(O)C(O)C2H5
	Pentan-2,3-dione
	Pentane-2,3-dione
Inchi:	InChI=1S/C5H8O2/c1-3-5(7)4(2)6/h3H2,1-2H3
InchiKey:	TZMFJUDUGYTVRY-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CCC(=O)C(C)=O
Mol. weight [g/mol]:	100.12
CAS:	600-14-6

Physical Properties

Property code	Value	Unit	Source
gf	-266.62	kJ/mol	Joback Method
hf	-371.69	kJ/mol	Joback Method
hfus	7.84	kJ/mol	Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure
hvap	40.22	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.554		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	681.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	681.00		NIST Webbook

rinpol	697.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	665.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	693.00	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	676.00	NIST Webbook
rinpol	673.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	663.00	NIST Webbook
rinpol	673.00	NIST Webbook
rinpol	652.00	NIST Webbook
rinpol	651.00	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	673.00	NIST Webbook
rinpol	664.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	664.00	NIST Webbook
rinpol	672.00	NIST Webbook
rinpol	709.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	668.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	694.00	NIST Webbook
rinpol	663.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	714.00	NIST Webbook
rinpol	665.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	720.00	NIST Webbook

rinpol	697.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	709.00	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	716.00	NIST Webbook
rinpol	707.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	668.00	NIST Webbook
rinpol	650.00	NIST Webbook
rinpol	664.00	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	665.00	NIST Webbook
rinpol	669.00	NIST Webbook
rinpol	666.00	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	703.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	693.00	NIST Webbook
rinpol	675.00	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	675.00	NIST Webbook

rinpol	660.00	NIST Webbook
rinpol	667.00	NIST Webbook
rinpol	653.00	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	667.00	NIST Webbook
ripol	1044.00	NIST Webbook
ripol	1034.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1062.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1062.00	NIST Webbook
ripol	1044.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1044.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1047.00	NIST Webbook
ripol	1026.00	NIST Webbook
ripol	1060.00	NIST Webbook
ripol	1044.00	NIST Webbook
ripol	1071.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1067.00	NIST Webbook
ripol	1052.00	NIST Webbook
ripol	1053.00	NIST Webbook
ripol	1062.00	NIST Webbook
ripol	1071.00	NIST Webbook
ripol	1069.00	NIST Webbook
ripol	1074.00	NIST Webbook
ripol	1074.00	NIST Webbook
ripol	1074.00	NIST Webbook
ripol	1040.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1054.00	NIST Webbook

ripol	1055.00	NIST Webbook
ripol	1049.00	NIST Webbook
ripol	1046.00	NIST Webbook
ripol	1051.00	NIST Webbook
ripol	1046.00	NIST Webbook
ripol	1044.00	NIST Webbook
ripol	1046.00	NIST Webbook
ripol	1026.00	NIST Webbook
ripol	1061.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1072.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1047.00	NIST Webbook
ripol	1059.00	NIST Webbook
ripol	1075.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1052.00	NIST Webbook
ripol	1052.00	NIST Webbook
ripol	1067.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1062.00	NIST Webbook
ripol	1063.00	NIST Webbook
ripol	1094.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1072.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1088.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1053.00	NIST Webbook
ripol	1043.00	NIST Webbook
ripol	1077.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1067.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1071.00	NIST Webbook
ripol	1055.00	NIST Webbook

ripol	1052.00	NIST Webbook
ripol	1066.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1102.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1067.00	NIST Webbook
ripol	1083.00	NIST Webbook
ripol	1054.00	NIST Webbook
ripol	1060.00	NIST Webbook
ripol	1064.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1079.00	NIST Webbook
ripol	1071.00	NIST Webbook
ripol	1070.00	NIST Webbook
ripol	1069.00	NIST Webbook
ripol	1076.00	NIST Webbook
ripol	1071.00	NIST Webbook
ripol	1071.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1064.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1040.00	NIST Webbook
ripol	1068.00	NIST Webbook
ripol	1064.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1080.00	NIST Webbook
ripol	1082.00	NIST Webbook
ripol	1076.00	NIST Webbook
ripol	1055.00	NIST Webbook
ripol	1076.00	NIST Webbook
ripol	1065.00	NIST Webbook
ripol	1063.00	NIST Webbook
ripol	1066.00	NIST Webbook
ripol	1066.00	NIST Webbook
ripol	1048.00	NIST Webbook
ripol	1065.00	NIST Webbook
ripol	1065.00	NIST Webbook
ripol	1038.00	NIST Webbook
ripol	1042.00	NIST Webbook
ripol	1064.00	NIST Webbook

ripol	1042.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1049.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1072.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	1061.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1062.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1055.00		NIST Webbook
ripol	1082.00		NIST Webbook
tb	384.20	K	NIST Webbook
tb	381.20	K	NIST Webbook
tc	613.03	K	Joback Method
tf	245.97	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.02	J/mol×K	613.03	Joback Method
cpg	164.27	J/mol×K	453.45	Joback Method
cpg	172.09	J/mol×K	485.37	Joback Method
cpg	179.57	J/mol×K	517.28	Joback Method
cpg	186.71	J/mol×K	549.20	Joback Method
cpg	193.52	J/mol×K	581.11	Joback Method
cpg	156.11	J/mol×K	421.54	Joback Method
dvisc	0.0004592	Pa×s	392.28	Joback Method
dvisc	0.0005966	Pa×s	363.02	Joback Method
dvisc	0.0008115	Pa×s	333.75	Joback Method
dvisc	0.0011710	Pa×s	304.49	Joback Method
dvisc	0.0018268	Pa×s	275.23	Joback Method
dvisc	0.0003666	Pa×s	421.54	Joback Method

dvisc	0.0031678	Pa×s	245.97	Joback Method
hfust	7.84	kJ/mol	221.20	NIST Webbook
pvap	45.32	kPa	358.85	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	55.21	kPa	364.69	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	60.20	kPa	367.09	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	65.19	kPa	369.44	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	70.18	kPa	371.61	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	75.27	kPa	373.80	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	40.33	kPa	355.74	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	35.34	kPa	352.15	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone

pvap	30.35	kPa	348.13	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	25.35	kPa	343.73	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	20.36	kPa	338.38	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	15.37	kPa	331.84	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
pvap	50.21	kPa	361.89	Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone
rhol	982.00	kg/m3	292.15	Vapor Liquid Equilibrium Data for 2,3-Pentanedione + (Acetaldehyde or Acetone) at (100, 150, and 200) kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45607e+01
Coeff. B	-3.35146e+03
Coeff. C	-4.71100e+01
Temperature range (K), min.	281.92
Temperature range (K), max.	409.46

Sources

Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure:	https://www.doi.org/10.1016/j.fluid.2006.02.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Liquid Equilibrium Data for 2,3-Pentanedione + (Acetaldehyde or Acetone) at (100, 150, and 200) K:	https://www.doi.org/10.1021/acs.jced.8b01196
Activity Coefficients at Infinite Dilution of Volatile Compounds in Water: Effect of Temperature and Salt Concentration:	https://www.doi.org/10.1021/je2013878
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C600146&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
Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone:	https://www.doi.org/10.1021/je7005924

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
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