2,3-Pentadione

Other names:	2,3-Pentandione
	2,3-pentanedione
	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
af	0.3979		Cheméo Relay (1.0)
gf	-266.62	kJ/mol	Joback Method
hf	-355.12	kJ/mol	Cheméo Relay (1.0)
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	43.26	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-0.04		Cheméo Relay (1.0)
logp	0.554		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	663.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	675.00		NIST Webbook
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ripol	1036.00		NIST Webbook
tb	384.20	K	NIST Webbook
tb	381.20	K	NIST Webbook
tc	601.28	K	Cheméo Relay (1.0)
tf	281.18	K	Cheméo Relay (1.0)
vc	0.329	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.02	J/mol×K	613.03	Joback Method
cpg	156.11	J/mol×K	421.54	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
dvisc	0.0008115	Pa×s	333.75	Joback Method
dvisc	0.0003666	Pa×s	421.54	Joback Method
dvisc	0.0004592	Pa×s	392.28	Joback Method
dvisc	0.0005966	Pa×s	363.02	Joback Method
dvisc	0.0011710	Pa×s	304.49	Joback Method
dvisc	0.0018268	Pa×s	275.23	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	50.21	kPa	361.89	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

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

Vapor Liquid Equilibrium for Binary Systems of 2,3-Pentanedione with Diacetyl and Acetone:	https://www.doi.org/10.1021/je7005924
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
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
Vapor Liquid Equilibrium Data for 2,3-Pentanedione + (Acetaldehyde or Acetone) at (100, 150, and 200) kPa:	https://www.doi.org/10.1021/acs.jced.8b01196
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C600146&Units=SI
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Activity Coefficients at Infinite Dilution of Volatile Compounds in Water: Effect of Temperature and Salt Concentration:	https://www.doi.org/10.1021/je2013878
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor

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
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
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