Pentanedioic acid, dimethyl ester

Other names:	Dimethyl glutarate
	Dimethyl pentanedioate
	Glutaric acid, dimethyl ester
	Methyl glutarate
Inchi:	InChI=1S/C7H12O4/c1-10-6(8)4-3-5-7(9)11-2/h3-5H2,1-2H3
InchiKey:	XTDYIOOONNVFMA-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	COC(=O)CCCC(=O)OC
Mol. weight [g/mol]:	160.17
CAS:	1119-40-0

Physical Properties

Property code	Value	Unit	Source
chs	-3612.00	kJ/mol	NIST Webbook
gf	-459.78	kJ/mol	Joback Method
hf	-677.41	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	65.70 ± 0.40	kJ/mol	NIST Webbook
hvap	66.10	kJ/mol	NIST Webbook
log10ws	-0.48		Crippen Method
logp	0.503		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	2770.00	kPa	Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids
rinpol	1104.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1139.80		NIST Webbook
rinpol	1108.00		NIST Webbook

rinpol	1134.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	189.90		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1107.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1687.00		NIST Webbook
tb	487.20	K	Liquid-Liquid Equilibria of Water + Acetic Acid + Dimethyl Glutarate Ternary System
tb	487.30	K	Liquid-Liquid Equilibria for Ternary Systems of Water + Formic Acid + Dibasic Esters
tc	697.87	K	Joback Method
tf	312.97	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.83	J/mol×K	635.96	Joback Method
cpg	335.29	J/mol×K	697.87	Joback Method
cpg	326.76	J/mol×K	666.91	Joback Method
cpg	278.30	J/mol×K	512.14	Joback Method
cpg	288.74	J/mol×K	543.09	Joback Method
cpg	298.81	J/mol×K	574.05	Joback Method
cpg	308.51	J/mol×K	605.00	Joback Method
dvisc	0.0003126	Pa×s	478.94	Joback Method
dvisc	0.0002482	Pa×s	512.14	Joback Method
dvisc	0.0005546	Pa×s	412.56	Joback Method
dvisc	0.0020676	Pa×s	312.97	Joback Method

dvisc	0.0012258	Pa×s	346.17	Joback Method
dvisc	0.0007964	Pa×s	379.36	Joback Method
dvisc	0.0004076	Pa×s	445.75	Joback Method
hvapt	54.70	kJ/mol	424.50	NIST Webbook
pvap	63.01	kPa	463.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	41.36	kPa	443.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	51.72	kPa	453.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	2.00	kPa	376.09	Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2, 5.2 and 8.3 kPa
pvap	5.20	kPa	395.80	Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2, 5.2 and 8.3 kPa

pvap	8.30	kPa	407.11	Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2, 5.2 and 8.3 kPa
pvap	8.85	kPa	393.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	19.14	kPa	413.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	19.10	kPa	413.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	25.31	kPa	423.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
pvap	32.89	kPa	433.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water

pvap	32.90	kPa	433.15	Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Dimethyl Adipate, Dimethyl Glutarate, Methanol, and Water
rfi	1.42454		293.15	(Liquid + liquid) equilibria of (water + propionic acid + dibasic esters) ternary systems
rfi	1.42454		293.15	(Liquid + liquid) equilibria of (water + butyric acid + dibasic esters) ternary systems
rfi	1.42454		293.15	Phase equilibria of (water + levulinic acid + dibasic esters) ternary systems

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	1.70	NIST Webbook
tbrp	376.50 ± 0.50	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72297e+01
Coeff. B	-5.94230e+03
Coeff. C	-1.59650e+01
Temperature range (K), min.	366.71
Temperature range (K), max.	514.55

Sources

Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2.5 kPa:	https://www.doi.org/10.1016/j.jct.2019.02.006
Vapor-Liquid Equilibrium of Mixtures Containing Adipic Acid, Glutaric Acid, Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je700027n
Dimethyl Adipate, Dimethyl Glutarate, and Dimethyl Succinate:	https://www.doi.org/10.1021/je0602418
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119400&Units=SI
Phase equilibria of (water + levulinic acid + dibasic esters) ternary systems:	https://www.doi.org/10.1016/j.fluid.2009.04.017
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
Liquid-Liquid Equilibria for Ternary Systems of Water + Formic Acid + Dibasic Esters:	https://www.doi.org/10.1021/je700206y
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-Liquid Equilibria of Water + Acetic Acid + Dimethyl Glutarate Ternary System:	https://www.doi.org/10.1021/je049571n
Liquid-liquid equilibria of aqueous mixtures containing selected dibasic esters and/or methanol:	https://www.doi.org/10.1016/j.fluid.2006.08.002
(Liquid + liquid) equilibria of the (water + carboxylic acid + dibasic esters mixture (DBE 2)) ternary systems:	https://www.doi.org/10.1016/j.fluid.2014.03.002
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
(Liquid + liquid) equilibria of (water + propionic acid + dibasic esters) ternary systems:	https://www.doi.org/10.1016/j.jct.2007.02.012
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
(Liquid + liquid) equilibria of (water + butyric acid + dibasic esters) ternary systems:	https://www.doi.org/10.1016/j.jct.2006.07.002
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume