Pentanedioic acid, diethyl ester

Other names:	DIETHYL GLUTARATE
	DIETHYL PENTANEDIOATE
	Ethyl glutarate
	Glutaric acid, diethyl ester
	Propane-1,3-dicarboxylic acid diethyl ester
	diethyl pentandioate
Inchi:	InChI=1S/C9H16O4/c1-3-12-8(10)6-5-7-9(11)13-4-2/h3-7H2,1-2H3
InchiKey:	OUWSNHWQZPEFEX-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	CCOC(=O)CCCC(=O)OCC
Mol. weight [g/mol]:	188.22
CAS:	818-38-2

Physical Properties

Property code	Value	Unit	Source
gf	-442.94	kJ/mol	Joback Method
hf	-718.69	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	53.94	kJ/mol	Joback Method
log10ws	-1.33		Aqueous Solubility Prediction Method
logp	1.283		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1282.10		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1292.00		NIST Webbook

rinpol	1284.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1780.00		NIST Webbook
tb	509.60	K	Liquid-liquid equilibria of (water + butyric acid + diethyl succinate or diethyl glutarate or diethyl adipate) ternary systems
tb	509.60	K	(Liquid + liquid) equilibria of (water + propionic acid + diethyl succinate or diethyl glutarate or diethyl adipate) ternary systems
tb	509.65	K	Liquid-Liquid Equilibria of (Water + Acetic Acid + Diethyl Succinate or Diethyl Glutarate or Diethyl Adipate) Ternary Systems
tb	510.20	K	NIST Webbook
tb	506.83	K	KDB
tc	682.00	K	Vapor-liquid critical temperatures and pressures of dicarboxylic acid diethyl esters
tf	249.05	K	Aqueous Solubility Prediction Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.00	J/mol×K	739.72	Joback Method
cpg	380.43	J/mol×K	588.20	Joback Method
cpg	392.33	J/mol×K	618.51	Joback Method
cpg	403.74	J/mol×K	648.81	Joback Method
cpg	414.66	J/mol×K	679.11	Joback Method
cpg	425.08	J/mol×K	709.42	Joback Method
cpg	368.05	J/mol×K	557.90	Joback Method
dvisc	0.0002660	Pa×s	520.84	Joback Method

dvisc	0.0003515	Pa×s	483.77	Joback Method
dvisc	0.0004864	Pa×s	446.70	Joback Method
dvisc	0.0007139	Pa×s	409.64	Joback Method
dvisc	0.0011310	Pa×s	372.57	Joback Method
dvisc	0.0002089	Pa×s	557.90	Joback Method
dvisc	0.0019834	Pa×s	335.51	Joback Method
hvapt	55.70	kJ/mol	424.00	NIST Webbook
pvap	0.02	kPa	318.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	322.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	323.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.04	kPa	328.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.06	kPa	333.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.09	kPa	338.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	0.12	kPa	343.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.17	kPa	347.90	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	313.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	311.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	8.77e-03	kPa	308.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	5.75e-03	kPa	303.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	3.52e-03	kPa	298.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

pvap	0.02	kPa	316.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	318.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76176e+01
Coeff. B	-6.43695e+03
Coeff. C	-1.11990e+01
Temperature range (K), min.	382.63
Temperature range (K), max.	534.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.84059e+01
Coeff. B	-7.19382e+03
Coeff. C	-1.58556e+00
Coeff. D	7.65275e-07
Temperature range (K), min.	338.15
Temperature range (K), max.	510.15

Sources

(Liquid + liquid) equilibria of (water + propionic acid + diethyl succinate or diethyl glutarate or diethyl adipate) ternary systems:	https://www.doi.org/10.1016/j.jct.2007.03.004
Vapor-liquid critical temperatures and pressures of dicarboxylic acid diethyl esters:	https://www.doi.org/10.1016/j.jct.2017.09.004

Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je100231g
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1109
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1109.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C818382&Units=SI
Liquid-liquid equilibria of (water + butyric acid + diethyl succinate or diethyl glutarate or diethyl adipate) ternary systems:	https://www.doi.org/10.1016/j.fluid.2011.01.012
Liquid-Liquid Equilibria of (Water + Acetic Acid + Diethyl Succinate or Diethyl Glutarate or Diethyl Adipate) Ternary Systems:	https://www.doi.org/10.1021/je7000733

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
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
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