Heptanedioic acid

Other names:	1,5-Pentanedicarboxylic acid
	1,7-Heptanedioic acid
	Heptandioic acid
	Heptane-1,7-dioic acid
	Pentane-1,5-dicarboxylic acid
	Pileric acid
	Pimelic acid
Inchi:	InChI=1S/C7H12O4/c8-6(9)4-2-1-3-5-7(10)11/h1-5H2,(H,8,9)(H,10,11)
InchiKey:	WLJVNTCWHIRURA-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	O=C(O)CCCCCC(=O)O
Mol. weight [g/mol]:	160.17
CAS:	111-16-0

Physical Properties

Property code	Value	Unit	Source
chs	-3460.20 ± 1.00	kJ/mol	NIST Webbook
gf	-523.42	kJ/mol	Joback Method
hf	-717.43	kJ/mol	Joback Method
hfus	1.50	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	139.90 ± 1.00	kJ/mol	NIST Webbook
hvap	112.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-0.25		Aqueous Solubility Prediction Method
logp	1.106		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3280.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
tb	651.66	K	Joback Method
tc	824.91	K	Joback Method
tf	377.50 ± 0.50	K	NIST Webbook
tf	378.48	K	Aqueous Solubility Prediction Method
tf	377.50 ± 0.40	K	NIST Webbook

tf	377.50 ± 0.30	K	NIST Webbook
tf	378.00 ± 1.50	K	NIST Webbook
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.31	J/mol×K	651.66	Joback Method
cpg	332.16	J/mol×K	680.54	Joback Method
cpg	339.63	J/mol×K	709.41	Joback Method
cpg	346.73	J/mol×K	738.29	Joback Method
cpg	353.47	J/mol×K	767.16	Joback Method
cpg	359.85	J/mol×K	796.04	Joback Method
cpg	365.90	J/mol×K	824.91	Joback Method
dvisc	0.0000300	Pa×s	651.66	Joback Method
dvisc	0.0013136	Pa×s	433.73	Joback Method
dvisc	0.0004681	Pa×s	477.32	Joback Method
dvisc	0.0046419	Pa×s	390.15	Joback Method
dvisc	0.0000959	Pa×s	564.49	Joback Method
dvisc	0.0000515	Pa×s	608.08	Joback Method
dvisc	0.0001983	Pa×s	520.90	Joback Method
hfust	23.70	kJ/mol	368.20	NIST Webbook
hfust	27.62	kJ/mol	377.50	NIST Webbook
hsubt	153.00 ± 4.00	kJ/mol	345.50	NIST Webbook
hsubt	124.00	kJ/mol	291.50	NIST Webbook
hsubt	80.80	kJ/mol	327.00	NIST Webbook
hsubt	178.00	kJ/mol	298.00	NIST Webbook
hvapt	88.60	kJ/mol	525.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.86116e+01
Coeff. B	-6.85336e+03
Coeff. C	-1.12189e+02
Temperature range (K), min.	486.20
Temperature range (K), max.	627.48

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.24988e+02
Coeff. B	-1.64286e+04
Coeff. C	-1.48852e+01
Coeff. D	5.07361e-06
Temperature range (K), min.	436.15
Temperature range (K), max.	615.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=966
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=966
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16:	https://www.doi.org/10.1016/j.jct.2004.12.011
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Reactive extraction of pimelic (heptanedioic) acid from dilute aqueous solutions using trioctylamine in decan-1-ol:	https://www.doi.org/10.1016/j.fluid.2016.02.039
An odd-even effect on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
Measurement and Correlation of Solubility of Pimelic Acid in Ether, Tetrahydrofuran, Ethanol, and Methanol:	https://www.doi.org/10.1021/je900629v
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111160&Units=SI

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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume