Decanedioic acid

Other names:	1,10-Decanedioic acid
	1,8-Octanedicarboxylic acid
	Decanedicarboxylic acid
	NSC 19492
	Sebacic acid
	Seracic acid
	USAF HC-1
	n-Decanedioic acid
Inchi:	InChI=1S/C10H18O4/c11-9(12)7-5-3-1-2-4-6-8-10(13)14/h1-8H2,(H,11,12)(H,13,14)
InchiKey:	CXMXRPHRNRROMY-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	O=C(O)CCCCCCCCC(=O)O
Mol. weight [g/mol]:	202.25
CAS:	111-20-6

Physical Properties

Property code	Value	Unit	Source
chs	-5425.00 ± 2.10	kJ/mol	NIST Webbook
gf	-498.16	kJ/mol	Joback Method
hf	-779.35	kJ/mol	Joback Method
hfus	44.90	kJ/mol	Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?
hfus	46.11	kJ/mol	Thermal analysis of phase change materials in the temperature range 120.150 .C
hfus	0.40	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	161.00 ± 3.00	kJ/mol	NIST Webbook
hvap	124.80	kJ/mol	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.276		Crippen Method
mcvol	166.640	ml/mol	McGowan Method

pc	2500.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
tb	720.30	K	Joback Method
tc	894.41	K	Joback Method
tf	407.00 ± 2.00	K	NIST Webbook
tf	406.90 ± 1.00	K	NIST Webbook
tf	404.00 ± 0.50	K	NIST Webbook
tf	405.00 ± 1.50	K	NIST Webbook
tf	404.00 ± 0.40	K	NIST Webbook
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.05	J/mol×K	778.34	Joback Method
cpg	473.58	J/mol×K	720.30	Joback Method
cpg	502.04	J/mol×K	807.35	Joback Method
cpg	510.57	J/mol×K	836.37	Joback Method
cpg	518.64	J/mol×K	865.39	Joback Method
cpg	526.27	J/mol×K	894.41	Joback Method
cpg	483.56	J/mol×K	749.32	Joback Method
dvisc	0.0006441	Pa×s	473.35	Joback Method
dvisc	0.0002289	Pa×s	522.74	Joback Method
dvisc	0.0000972	Pa×s	572.13	Joback Method
dvisc	0.0000473	Pa×s	621.52	Joback Method
dvisc	0.0000256	Pa×s	670.91	Joback Method
dvisc	0.0023069	Pa×s	423.96	Joback Method
dvisc	0.0000151	Pa×s	720.30	Joback Method
hfust	40.80	kJ/mol	404.00	NIST Webbook
hfust	46.60	kJ/mol	403.90	NIST Webbook
hfust	45.30	kJ/mol	405.60	NIST Webbook
hfust	46.90	kJ/mol	405.70	NIST Webbook
hfust	40.81	kJ/mol	404.00	NIST Webbook
hfust	40.80	kJ/mol	404.00	NIST Webbook
hsubt	160.70 ± 2.50	kJ/mol	389.00	NIST Webbook
hsubt	146.50	kJ/mol	311.00	NIST Webbook
hsubt	181.00 ± 8.00	kJ/mol	369.00	NIST Webbook
hvapt	85.90	kJ/mol	540.50	NIST Webbook
sfust	101.00	J/mol×K	404.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	546.20	K	6.70	NIST Webbook
tbrp	568.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69408e+01
Coeff. B	-6.61985e+03
Coeff. C	-1.10231e+02
Temperature range (K), min.	507.74
Temperature range (K), max.	679.47

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356
Solubility of decanedioic acid in binary solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2011.02.018
Measurement and Correlation of Solubilities of Decanedioic Acid in C4−C6 Alcohol Solvents:	https://www.doi.org/10.1021/je900587b
Thermal analysis of phase change materials in the temperature range 120-150° C:	https://www.doi.org/10.1016/j.tca.2010.11.011
Solubility of Sebacic Acid in Binary Mixtures Containing Alcohols:	https://www.doi.org/10.1021/je800549f
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Sebacic Acid in Binary Water + Ethanol Solvent Mixtures:	https://www.doi.org/10.1021/je7005314
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
An odd-even effect on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111206&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?:	https://www.doi.org/10.1016/j.tca.2014.09.022

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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume