Nonanedioic acid

Other names:	1,7-Dicarboxyheptane
	1,7-Heptanedicarboxylic acid
	1,9-nonanedioic acid
	Anchoic acid
	Azelaic acid, technical grade
	Azelainic acid
	Emerox 1110
	Emerox 1144
	Emery's L-110
	Finacea
	Heptanedicarboxylic acid
	Lepargylic acid
	NSC 19493
	Skinoren
	ZK-62498
	azelaic acid
	n-Nonanedioic acid
Inchi:	InChI=1S/C9H16O4/c10-8(11)6-4-2-1-3-5-7-9(12)13/h1-7H2,(H,10,11)(H,12,13)
InchiKey:	BDJRBEYXGGNYIS-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	O=C(O)CCCCCCCC(=O)O
Mol. weight [g/mol]:	188.22

Physical Properties

Property code	Value	Unit	Source
af	0.9582		Cheméo Relay (1.0)
chs	-4773.90 ± 1.90	kJ/mol	NIST Webbook
chs	-4775.60	kJ/mol	NIST Webbook
chs	-4773.90 ± 1.90	kJ/mol	NIST Webbook
gf	-506.58	kJ/mol	Joback Method
hf	-905.36	kJ/mol	Cheméo Relay (1.0)
hfs	-1054.30 ± 0.90	kJ/mol	NIST Webbook
hfus	0.01	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	159.90 ± 1.00	kJ/mol	NIST Webbook
hvap	119.70 ± 0.80	kJ/mol	NIST Webbook

ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-1.89		Aqueous Solubility Prediction Method
logp	1.886		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2720.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
rinpol	1672.20		NIST Webbook
rinpol	1672.20		NIST Webbook
tb	552.67	K	Cheméo Relay (1.0)
tc	770.16	K	Cheméo Relay (1.0)
tf	379.70 ± 1.00	K	NIST Webbook
tf	380.00 ± 0.50	K	NIST Webbook
tf	375.60	K	Solid-Liquid Equilibria of Nonanedioic Acid in Binary Ethanol + Water Solvent Mixtures from (292.35 to 345.52) K
vc	0.574	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.66	J/mol×K	870.76	Joback Method
cpg	422.42	J/mol×K	697.42	Joback Method
cpg	431.74	J/mol×K	726.31	Joback Method
cpg	440.59	J/mol×K	755.20	Joback Method
cpg	449.00	J/mol×K	784.09	Joback Method
cpg	456.97	J/mol×K	812.98	Joback Method
cpg	464.52	J/mol×K	841.87	Joback Method
dvisc	0.0000598	Pa×s	602.51	Joback Method
dvisc	0.0008162	Pa×s	460.15	Joback Method
dvisc	0.0002902	Pa×s	507.60	Joback Method
dvisc	0.0001231	Pa×s	555.06	Joback Method
dvisc	0.0000323	Pa×s	649.96	Joback Method
dvisc	0.0000189	Pa×s	697.42	Joback Method
dvisc	0.0029117	Pa×s	412.69	Joback Method
hfust	32.68	kJ/mol	380.00	NIST Webbook
hfust	32.67	kJ/mol	380.00	NIST Webbook
hfust	32.67	kJ/mol	380.00	NIST Webbook
hfust	29.70	kJ/mol	372.40	NIST Webbook

hfust	35.30	kJ/mol	375.60	NIST Webbook
hsubt	178.00 ± 5.00	kJ/mol	360.50	NIST Webbook
hsubt	156.20 ± 0.50	kJ/mol	372.00	NIST Webbook
hsubt	138.00	kJ/mol	302.50	NIST Webbook
hvapt	89.30	kJ/mol	540.50	NIST Webbook
sfust	85.98	J/mol×K	380.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	560.20	K	13.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356
Solubility of Azelaic Acid in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je600572z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
An odd-even effect on solubility of dicarboxylic acids in organic solvents:	https://www.doi.org/10.1016/j.jct.2014.05.009
Solid-Liquid Equilibria of Nonanedioic Acid in Binary Ethanol + Water Solvent Mixtures from (292.35 to 345.52) K:	https://www.doi.org/10.1021/je800921n
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123999&Units=SI
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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

af:	Acentric Factor
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

hfs:	Solid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
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