Undecanedioic acid

Other names:	1,11-Undecanedioic acid
	1,9-Nonanedicarboxylic acid
	Undecanedionic acid
Inchi:	InChI=1S/C11H20O4/c12-10(13)8-6-4-2-1-3-5-7-9-11(14)15/h1-9H2,(H,12,13)(H,14,15)
InchiKey:	LWBHHRRTOZQPDM-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	O=C(O)CCCCCCCCCC(=O)O
Mol. weight [g/mol]:	216.27
CAS:	1852-04-6

Physical Properties

Property code	Value	Unit	Source
chs	-6087.50 ± 2.50	kJ/mol	NIST Webbook
gf	-489.74	kJ/mol	Joback Method
hf	-799.99	kJ/mol	Joback Method
hfus	1.60	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	162.50 ± 1.90	kJ/mol	NIST Webbook
hvap	128.20 ± 2.30	kJ/mol	NIST Webbook
log10ws	-2.63		Crippen Method
logp	2.667		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	743.18	K	Joback Method
tc	918.61	K	Joback Method
tf	385.00 ± 9.47	K	NIST Webbook
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.03	J/mol×K	743.18	Joback Method
cpg	546.73	J/mol×K	801.66	Joback Method

cpg	582.00	J/mol×K	918.61	Joback Method
cpg	556.29	J/mol×K	830.89	Joback Method
cpg	565.34	J/mol×K	860.13	Joback Method
cpg	573.90	J/mol×K	889.37	Joback Method
cpg	536.65	J/mol×K	772.42	Joback Method
dvisc	0.0000204	Pa×s	691.86	Joback Method
dvisc	0.0000375	Pa×s	640.53	Joback Method
dvisc	0.0000769	Pa×s	589.20	Joback Method
dvisc	0.0001808	Pa×s	537.88	Joback Method
dvisc	0.0005089	Pa×s	486.56	Joback Method
dvisc	0.0000120	Pa×s	743.18	Joback Method
dvisc	0.0018288	Pa×s	435.23	Joback Method
hfust	39.65	kJ/mol	385.00	NIST Webbook
hfust	39.65	kJ/mol	385.00	NIST Webbook
hfust	41.20	kJ/mol	380.10	NIST Webbook
hfust	39.65	kJ/mol	385.00	NIST Webbook
hsubt	158.60 ± 1.90	kJ/mol	376.00	NIST Webbook
hsubt	141.50	kJ/mol	304.00	NIST Webbook
sfust	103.00	J/mol×K	385.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60635e+01
Coeff. B	-6.18724e+03
Coeff. C	-1.21875e+02
Temperature range (K), min.	514.07
Temperature range (K), max.	697.33

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C24 and C16: https://www.doi.org/10.1016/j.jct.2004.12.011

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1852046&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume