Dodecanedioic acid

Other names:	1,10-Decanedicarboxylic acid
	1,10-decandicarboxylic acid
	1,12-Dodecanedioic acid
	Decamethylenedicarboxylic acid
	Dodecanedicarboxylic acid
Inchi:	InChI=1S/C12H22O4/c13-11(14)9-7-5-3-1-2-4-6-8-10-12(15)16/h1-10H2,(H,13,14)(H,15,
InchiKey:	TVIDDXQYHWJXFK-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	O=C(O)CCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	230.30
CAS:	693-23-2

Physical Properties

Property code	Value	Unit	Source
chs	-6736.20 ± 2.80	kJ/mol	NIST Webbook
gf	-481.32	kJ/mol	Joback Method
hf	-820.63	kJ/mol	Joback Method
hfus	0.06	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hsub	153.00 ± 3.00	kJ/mol	NIST Webbook
hvap	130.00 ± 2.30	kJ/mol	NIST Webbook
log10ws	-3.04		Crippen Method
logp	3.057		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	2150.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
tb	766.06	K	Joback Method
tc	943.42	K	Joback Method
tf	402.50 ± 0.50	K	NIST Webbook
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.68	J/mol×K	766.06	Joback Method
cpg	590.93	J/mol×K	795.62	Joback Method
cpg	601.59	J/mol×K	825.18	Joback Method
cpg	611.69	J/mol×K	854.74	Joback Method
cpg	621.24	J/mol×K	884.30	Joback Method
cpg	630.27	J/mol×K	913.86	Joback Method
cpg	638.80	J/mol×K	943.42	Joback Method
dvisc	0.0000096	Pa×s	766.06	Joback Method
dvisc	0.0004026	Pa×s	499.76	Joback Method
dvisc	0.0001430	Pa×s	553.02	Joback Method
dvisc	0.0000609	Pa×s	606.28	Joback Method
dvisc	0.0014511	Pa×s	446.50	Joback Method
dvisc	0.0000162	Pa×s	712.80	Joback Method
dvisc	0.0000298	Pa×s	659.54	Joback Method
hfust	50.56	kJ/mol	402.50	NIST Webbook
hfust	52.50	kJ/mol	401.60	NIST Webbook
hfust	49.80	kJ/mol	400.30	NIST Webbook
hfust	50.57	kJ/mol	402.50	NIST Webbook
hsubt	169.00 ± 4.00	kJ/mol	361.50	NIST Webbook
hsubt	156.00	kJ/mol	307.00	NIST Webbook
hsubt	153.10 ± 2.90	kJ/mol	335.50	NIST Webbook
sfust	125.60	J/mol×K	402.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	518.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56665e+01
Coeff. B	-6.09579e+03
Coeff. C	-1.24099e+02
Temperature range (K), min.	520.47
Temperature range (K), max.	712.78

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and correlation of solubility of dodecanedioic acid in different pure solvents from T = (288.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2013.09.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693232&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
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