

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)CCCCCCCCC(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.80	J/molxK	943.42	Joback Method
cpg	579.68	J/molxK	766.06	Joback Method
cpg	590.93	J/molxK	795.62	Joback Method
cpg	601.59	J/molxK	825.18	Joback Method
cpg	611.69	J/molxK	854.74	Joback Method
cpg	621.24	J/molxK	884.30	Joback Method
cpg	630.27	J/molxK	913.86	Joback Method
dvisc	0.0000096	Paxs	766.06	Joback Method
dvisc	0.0014511	Paxs	446.50	Joback Method
dvisc	0.0004026	Paxs	499.76	Joback Method
dvisc	0.0001430	Paxs	553.02	Joback Method
dvisc	0.0000609	Paxs	606.28	Joback Method
dvisc	0.0000298	Paxs	659.54	Joback Method
dvisc	0.0000162	Paxs	712.80	Joback Method
hfust	50.57	kJ/mol	402.50	NIST Webbook
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
hsubt	153.10 ± 2.90	kJ/mol	335.50	NIST Webbook
hsubt	169.00 ± 4.00	kJ/mol	361.50	NIST Webbook
hsubt	156.00	kJ/mol	307.00	NIST Webbook
sfust	125.60	J/molxK	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	$\ln(P_{vp}) = A + B/(T + C)$
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

The Yaws Handbook of Vapor Pressure: Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C1 to C16:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Measurement and correlation of solubility of dodecanedioic acid in different solvents from T = (288.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2013.09.012
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C1 to C14):	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693232&Units=SI
	https://www.doi.org/10.1021/je0498356
	https://www.chemeo.com/doc/models/crippen_log10ws

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

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