1,10-Decanediol

Other names:	1,10-Decamethylene diol
	1,10-Decamethylene glycol
	1,10-Dihydroxydecane
	1,6-Bis(2-hydroxyethyl)hexane
	Decamethylene glycol
	Decamethylenediol
	Decane-1,10-diol
	NSC 17165
	«alpha»,«omega»-Decanediol
	Â«alphaÂ»,Â«omegaÂ»-Decanediol
Inchi:	InChI=1S/C10H22O2/c11-9-7-5-3-1-2-4-6-8-10-12/h11-12H,1-10H2
InchiKey:	FOTKYAAJKYLFFN-UHFFFAOYSA-N
Formula:	C10H22O2
SMILES:	OCCCCCCCCCCO
Mol. weight [g/mol]:	174.28
CAS:	112-47-0

Physical Properties

Property code	Value	Unit	Source
chs	-6386.00 ± 3.00	kJ/mol	NIST Webbook
chs	-6400.30 ± 2.20	kJ/mol	NIST Webbook
gf	-240.32	kJ/mol	Joback Method
hf	-537.80	kJ/mol	NIST Webbook
hf	-523.10 ± 2.50	kJ/mol	NIST Webbook
hfs	-693.58	kJ/mol	NIST Webbook
hfs	-678.90 ± 2.30	kJ/mol	NIST Webbook
hfus	44.96	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?
hsub	155.80 ± 0.90	kJ/mol	NIST Webbook
hsub	155.80	kJ/mol	NIST Webbook
hsub	155.80 ± 0.90	kJ/mol	NIST Webbook
hvap	126.60 ± 4.20	kJ/mol	NIST Webbook
hvap	113.70 ± 2.10	kJ/mol	NIST Webbook

hvap	120.40 ± 4.90	kJ/mol	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.092		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	612.56	K	Joback Method
tc	770.00	K	Critical temperatures and pressures of straight-chain alkanediols (C3 to C12)
tf	345.70 ± 0.20	K	NIST Webbook
tf	345.40 ± 1.00	K	NIST Webbook
tf	343.30 ± 0.30	K	NIST Webbook
tf	344.15 ± 2.00	K	NIST Webbook
tf	345.80 ± 1.00	K	NIST Webbook
tf	345.80	K	Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect
tt	345.40 ± 0.10	K	NIST Webbook
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.57	J/mol×K	612.56	Joback Method
cpg	453.22	J/mol×K	638.77	Joback Method
cpg	464.40	J/mol×K	664.99	Joback Method
cpg	475.14	J/mol×K	691.20	Joback Method
cpg	485.44	J/mol×K	717.42	Joback Method
cpg	495.33	J/mol×K	743.63	Joback Method
cpg	504.80	J/mol×K	769.84	Joback Method
dvisc	0.0009280	Pa×s	420.25	Joback Method
dvisc	0.0039246	Pa×s	372.18	Joback Method
dvisc	0.0254585	Pa×s	324.10	Joback Method
dvisc	0.0002950	Pa×s	468.33	Joback Method
dvisc	0.0001161	Pa×s	516.41	Joback Method
dvisc	0.0000536	Pa×s	564.48	Joback Method
dvisc	0.0000279	Pa×s	612.56	Joback Method

hfust	41.70	kJ/mol	345.50	NIST Webbook
hfust	41.70	kJ/mol	345.50	NIST Webbook
hvapt	120.00	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography
hvapt	112.40	kJ/mol	364.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	1.00	NIST Webbook
tbrp	443.00	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.12348e+01
Coeff. B	-7.23679e+03
Coeff. C	-1.00722e+02
Temperature range (K), min.	446.20
Temperature range (K), max.	555.20

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-alpha,omega-diols	https://www.doi.org/10.1016/j.jct.2013.08.019
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
HO-CH2-n-OH: Structure-related odd even effect.	https://www.doi.org/10.1021/je060333x
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.doi.org/10.1016/j.tca.2014.09.022
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://en.wikipedia.org/wiki/Joback_method
Joback Method:	https://www.doi.org/10.1016/j.fluid.2013.06.048
Critical temperatures and pressures of straight-chain alkanediols (C3 to C12):	

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112470&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
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume