

1,12-Dodecanediol

Other names:	1,12-dihydroxydodecane Dodecamethylene glycol dodecane-1,12-diol n-dodecane-1,12-diol
Inchi:	InChI=1S/C12H26O2/c13-11-9-7-5-3-1-2-4-6-8-10-12-14/h13-14H,1-12H2
InchiKey:	GHLKSLMMWAKNBM-UHFFFAOYSA-N
Formula:	C12H26O2
SMILES:	OCCCCCCCCCCCCO
Mol. weight [g/mol]:	202.33
CAS:	5675-51-4

Physical Properties

Property code	Value	Unit	Source
gf	-223.48	kJ/mol	Joback Method
hf	-595.47	kJ/mol	Joback Method
hfus	35.01	kJ/mol	Joback Method
hvap	75.66	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.872		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	658.32	K	Joback Method
tc	798.00	K	Critical temperatures and pressures of straight-chain alkanediols (C3 to C12)
tf	352.90	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
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.33	J/molxK	791.00	Joback Method
cpg	593.37	J/molxK	764.46	Joback Method
cpg	581.92	J/molxK	737.93	Joback Method
cpg	569.97	J/molxK	711.39	Joback Method
cpg	557.50	J/molxK	684.86	Joback Method
cpg	544.50	J/molxK	658.32	Joback Method
cpg	614.83	J/molxK	817.53	Joback Method
dvisc	0.0133348	Paxs	346.64	Joback Method
dvisc	0.0000170	Paxs	658.32	Joback Method
dvisc	0.0000321	Paxs	606.37	Joback Method
dvisc	0.0000682	Paxs	554.43	Joback Method
dvisc	0.0001694	Paxs	502.48	Joback Method
dvisc	0.0005191	Paxs	450.53	Joback Method
dvisc	0.0021293	Paxs	398.59	Joback Method
hfust	51.20	kJ/mol	352.00	NIST Webbook
hvapt	135.00	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	462.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.26296e+01
Coeff. B	-8.02364e+03

Coeff. C	-1.07992e+02
Temperature range (K), min.	467.12
Temperature range (K), max.	571.30

Sources

Thermodynamics of fusion and sublimation for a homologous series of even-alkane α,ω -diols Joback Method:	https://www.doi.org/10.1016/j.jct.2013.08.019
HO-(CH ₂) _n -OH: Structure-related odd even effect. McGowan Method:	https://en.wikipedia.org/wiki/Joback_method http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure: NIST Webbook:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure http://webbook.nist.gov/cgi/cbook.cgi?ID=C5675514&Units=SI
Critical temperatures and pressures of straight-chain alkanediols (C3 to C12): Crippen Method:	https://www.doi.org/10.1016/j.fluid.2013.06.048 http://pubs.acs.org/doi/abs/10.1021/ci9903071
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Crippen Method:	https://www.doi.org/10.1021/je060333x https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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
vc:	Critical Volume

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