

# (S)-(+)-1,2-Propanediol

<b>Other names:</b>	(+)-(S)-1,2-propanediol (+)-1,2-propanediol (S)-1,2-propanediol (S)-Propylene glycol 1,2-(S)-propanediol 1,2-Propanediol, (S)- 1,2-propanediol, (S)-(+)- 3-deoxy-sn-glycerol L(+)-propanediol L-(+)-1,2-propanediol L-(+)-propylene glycol L-1,2-propanediol S(+)-propane-1,2-diol S-(+)-Propylene glycol d-propylene glycol propylene glycol, (S)-(+)-
<b>Inchi:</b>	InChI=1S/C3H8O2/c1-3(5)2-4/h3-5H,2H2,1H3/t3-/m0/s1
<b>InchiKey:</b>	DNIAPMSPWPWGF-VKHMYYHEASA-N
<b>Formula:</b>	C3H8O2
<b>SMILES:</b>	CC(O)CO
<b>Mol. weight [g/mol]:</b>	76.09
<b>CAS:</b>	4254-15-3

## Physical Properties

Property code	Value	Unit	Source
gf	-301.70	kJ/mol	Joback Method
hf	-414.99	kJ/mol	Joback Method
hfus	8.18	kJ/mol	Joback Method
hvap	69.20 ± 0.30	kJ/mol	NIST Webbook
log10ws	0.28		Crippen Method
logp	-0.640		Crippen Method
mcvol	64.870	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
tb	451.96	K	Joback Method
tc	614.38	K	Joback Method
tf	230.21	K	Joback Method
vc	0.235	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.24	J/molxK	614.38	Joback Method
cpg	140.93	J/molxK	479.03	Joback Method
cpg	146.19	J/molxK	506.10	Joback Method
cpg	151.24	J/molxK	533.17	Joback Method
cpg	156.10	J/molxK	560.24	Joback Method
cpg	160.76	J/molxK	587.31	Joback Method
cpg	135.47	J/molxK	451.96	Joback Method
dvisc	0.0001649	Paxs	451.96	Joback Method
dvisc	0.0003678	Paxs	415.00	Joback Method
dvisc	0.9647802	Paxs	230.21	Joback Method
dvisc	0.0009593	Paxs	378.04	Joback Method
dvisc	0.0030803	Paxs	341.08	Joback Method
dvisc	0.0131321	Paxs	304.13	Joback Method
dvisc	0.0836198	Paxs	267.17	Joback Method
hfust	8.40	kJ/mol	240.00	NIST Webbook
pvap	6.85e-03	kPa	288.20	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.02	kPa	301.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.02	kPa	303.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.03	kPa	303.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.03	kPa	305.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.04	kPa	306.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.04	kPa	306.40	1,2-Propanediol. Comprehensive experimental and theoretical study

pvap	0.05	kPa	309.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.05	kPa	310.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.04	kPa	310.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.04	kPa	310.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.06	kPa	312.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.06	kPa	312.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.07	kPa	313.20	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.07	kPa	313.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.05	kPa	313.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.07	kPa	315.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.09	kPa	316.20	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.09	kPa	316.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.09	kPa	316.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.10	kPa	318.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.09	kPa	318.40	1,2-Propanediol. Comprehensive experimental and theoretical study

pvap	0.11	kPa	319.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.12	kPa	320.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.10	kPa	320.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.10	kPa	320.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.13	kPa	321.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.14	kPa	322.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.14	kPa	322.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.13	kPa	323.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.16	kPa	323.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.13	kPa	323.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.13	kPa	324.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.17	kPa	325.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.14	kPa	325.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.17	kPa	325.40	1,2-Propanediol. Comprehensive experimental and theoretical study

pvap	0.18	kPa	326.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.15	kPa	326.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.17	kPa	327.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.20	kPa	327.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.22	kPa	328.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.18	kPa	328.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.18	kPa	328.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.22	kPa	328.60	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.24	kPa	329.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.28	kPa	331.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.23	kPa	331.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.03	kPa	301.30	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.30	kPa	335.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.37	kPa	338.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.02	kPa	298.40	1,2-Propanediol. Comprehensive experimental and theoretical study

pvap	0.02	kPa	298.20	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.01	kPa	297.40	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	9.68e-03	kPa	293.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.01	kPa	293.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	4.27e-03	kPa	283.50	1,2-Propanediol. Comprehensive experimental and theoretical study
pvap	0.26	kPa	333.30	1,2-Propanediol. Comprehensive experimental and theoretical study

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	460.20	K	102.00	NIST Webbook

## Sources

1,2-Propanediol. Comprehensive experimental and theoretical study:  
Joback Method:

<https://www.doi.org/10.1016/j.jct.2009.04.019>

[https://en.wikipedia.org/wiki/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=C4254153&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/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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