Propane-1,3-diol, 2-methyl-

Other names:	1,3-Propanediol, 2-methyl-
	1,3-dihydroxyisobutane
	2-Methyl-1,3-propanediol
	2-methylpropane-1,3-diol
	MP diol glycol
	propanediol 2-methyl
Inchi:	InChI=1S/C4H10O2/c1-4(2-5)3-6/h4-6H,2-3H2,1H3
InchiKey:	QWGRWMMWNDWRQN-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CC(CO)CO
Mol. weight [g/mol]:	90.12
CAS:	2163-42-0

Physical Properties

Property code	Value	Unit	Source
gf	-293.28	kJ/mol	Joback Method
hf	-435.63	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	73.60 ± 0.20	kJ/mol	NIST Webbook
hvap	71.30 ± 0.50	kJ/mol	NIST Webbook
log10ws	0.22		Crippen Method
logp	-0.393		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	474.84	K	Joback Method
tc	636.47	K	Joback Method
tf	241.48	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.31	J/mol×K	474.84	Joback Method
cpg	179.93	J/mol×K	501.78	Joback Method

cpg	186.29	J/mol×K	528.72	Joback Method
cpg	192.41	J/mol×K	555.66	Joback Method
cpg	198.29	J/mol×K	582.59	Joback Method
cpg	203.94	J/mol×K	609.53	Joback Method
cpg	209.35	J/mol×K	636.47	Joback Method
dvisc	0.6060212	Pa×s	241.48	Joback Method
dvisc	0.0554139	Pa×s	280.37	Joback Method
dvisc	0.0090753	Pa×s	319.27	Joback Method
dvisc	0.0022017	Pa×s	358.16	Joback Method
dvisc	0.0007050	Pa×s	397.05	Joback Method
dvisc	0.0002766	Pa×s	435.95	Joback Method
dvisc	0.0001265	Pa×s	474.84	Joback Method
pvap	0.01	kPa	316.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	2.85e-03	kPa	300.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	3.64e-03	kPa	303.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	4.90e-03	kPa	306.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	6.61e-03	kPa	309.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	8.41e-03	kPa	312.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	8.61e-03	kPa	312.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	9.96e-03	kPa	314.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

pvap	2.04e-03	kPa	297.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.01	kPa	318.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	319.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	321.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	322.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	323.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.02	kPa	323.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.03	kPa	326.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.03	kPa	326.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.03	kPa	328.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.03	kPa	328.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.04	kPa	331.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

pvap	0.05	kPa	333.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.06	kPa	336.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.07	kPa	338.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.09	kPa	341.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.09	kPa	342.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.11	kPa	343.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.14	kPa	347.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.16	kPa	349.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.19	kPa	352.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.24	kPa	355.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols
pvap	0.26	kPa	357.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.87497e+01
Coeff. B	-5.54127e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	376.72
Temperature range (K), max.	488.93

Sources

Vapor Pressures and Enthalpies of Vaporization of a Series of the 1,3-Alkanediols:	https://www.doi.org/10.1021/je060419q
Partial Molar Isentropic Compressions and Partial Molar Volumes of Selected Branched Aliphatic Alcohols at Infinite Dilution in Water at Temperatures from T = (278 to 318) K and Atmospheric Pressure:	https://www.doi.org/10.1021/je300175w
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=C2163420&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/ci990307l
Crippen Method:	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
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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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