1,3-Propanediol, 2-methyl-2-propyl-

Other names:	2-Methyl-2-n-propyl-1,3-propanediol
	2-Methyl-2-propyl-1,3-propanediol
	2-methyl-2-propylpropane-1,3-diol
Inchi:	InChI=1S/C7H16O2/c1-3-4-7(2,5-8)6-9/h8-9H,3-6H2,1-2H3
InchiKey:	JVZZUPJFERSVRN-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCCC(C)(CO)CO
Mol. weight [g/mol]:	132.20
CAS:	78-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-262.74	kJ/mol	Joback Method
hf	-501.02	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.777		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	540.69	K	Joback Method
tc	705.20	K	Joback Method
tf	328.90 ± 0.60	K	NIST Webbook
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.55	J/mol×K	540.69	Joback Method
cpg	312.41	J/mol×K	568.11	Joback Method
cpg	321.81	J/mol×K	595.53	Joback Method
cpg	330.76	J/mol×K	622.94	Joback Method
cpg	339.28	J/mol×K	650.36	Joback Method
cpg	347.40	J/mol×K	677.78	Joback Method

cpg	355.13	J/mol×K	705.20	Joback Method
dvisc	0.0841554	Pa×s	292.71	Joback Method
dvisc	0.0117921	Pa×s	334.04	Joback Method
dvisc	0.0025471	Pa×s	375.37	Joback Method
dvisc	0.0007456	Pa×s	416.70	Joback Method
dvisc	0.0002724	Pa×s	458.03	Joback Method
dvisc	0.0001176	Pa×s	499.36	Joback Method
dvisc	0.0000577	Pa×s	540.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67442e+01
Coeff. B	-5.13431e+03
Coeff. C	-8.28880e+01
Temperature range (K), min.	394.88
Temperature range (K), max.	531.98

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solubility of 2-methyl-2-propyl-1,3-propanediol and its derivatives in supercritical carbon dioxide: measurement and mathematical modeling: https://www.doi.org/10.1016/j.jct.2013.06.015

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=C78262&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume