2-Ethyl-2-methyl-1,3-propanediol

Other names: 1,3-Propanediol, 2-ethyl-2-methyl-
2-Methyl-2-ethyl-1,3-propanediol
2-ethyl-2-methylpropane-1,3-diol
Inchi: InChI=1S/C6H14O2/c1-3-6(2,4-7)5-8/h7-8H,3-5H2,1-2H3
InchiKey: VNAWKNVDKFZFSU-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCC(C)(CO)CO
Mol. weight [g/mol]: 118.17
CAS: 77-84-9

Physical Properties

Property code	Value	Unit	Source
gf	-271.16	kJ/mol	Joback Method
hf	-480.38	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	61.01	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	0.387		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	499.00	K	NIST Webbook
tb	498.95	K	NIST Webbook
tc	683.21	K	Joback Method
tf	313.45	K	NIST Webbook
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.59	J/mol×K	517.81	Joback Method
cpg	267.62	J/mol×K	545.38	Joback Method
cpg	276.20	J/mol×K	572.94	Joback Method
cpg	284.37	J/mol×K	600.51	Joback Method
cpg	292.14	J/mol×K	628.08	Joback Method

cpg	299.53	J/mol×K	655.65	Joback Method
cpg	306.56	J/mol×K	683.21	Joback Method
dvisc	0.1240865	Pa×s	281.44	Joback Method
dvisc	0.0170071	Pa×s	320.83	Joback Method
dvisc	0.0036001	Pa×s	360.23	Joback Method
dvisc	0.0010350	Pa×s	399.62	Joback Method
dvisc	0.0003722	Pa×s	439.02	Joback Method
dvisc	0.0001584	Pa×s	478.41	Joback Method
dvisc	0.0000768	Pa×s	517.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63740e+01
Coeff. B	-4.92730e+03
Coeff. C	-7.98580e+01
Temperature range (K), min.	386.16
Temperature range (K), max.	525.26

Sources

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=C77849&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