

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:	VNAWKNVDFKZFSU-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	498.95	K	NIST Webbook
tb	499.00	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/molxK	517.81	Joback Method
cpg	267.62	J/molxK	545.38	Joback Method
cpg	276.20	J/molxK	572.94	Joback Method
cpg	284.37	J/molxK	600.51	Joback Method
cpg	292.14	J/molxK	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	Paxs	281.44	Joback Method
dvisc	0.0170071	Paxs	320.83	Joback Method
dvisc	0.0036001	Paxs	360.23	Joback Method
dvisc	0.0010350	Paxs	399.62	Joback Method
dvisc	0.0003722	Paxs	439.02	Joback Method
dvisc	0.0001584	Paxs	478.41	Joback Method
dvisc	0.0000768	Paxs	517.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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/ci9903071

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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