1,3-Hexanediol, 2-ethyl-

Other names:	2-Ethyl-1,3-hexandiol
	2-Ethyl-1,3-hexanediol
	2-Ethyl-1,3-hexylene glycol
	2-Ethyl-3-propyl-1,3-propanediol
	2-Ethylhexane-1,3-diol
	2-Ethylhexanediol
	2-Ethylhexanediol-1,3
	3-Hydroxymethyl-n-heptan-4-ol
	6-12
	6-12-Insect repellent
	Carbide 6-12
	Compound 6-12, insect repellent
	Diol-Kyowa 8
	EH diol
	EHD
	ENT 375
	Ethohexadiol
	Ethyl hexanediol
	Ethyl hexylene glycol
	Ethyl-1,3-hexane diol-2
	NSC 3881
	Octylene glycol
	Repellent 612
	Rutgers 612
Inchi:	InChI=1S/C8H18O2/c1-3-5-8(10)7(4-2)6-9/h7-10H,3-6H2,1-2H3
InchiKey:	RWLALWYNXFYRGW-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CCCC(O)C(CC)CO
Mol. weight [g/mol]:	146.23
CAS:	94-96-2

Physical Properties

Property code	Value	Unit	Source
gf	-262.04	kJ/mol	Joback Method
hf	-523.47	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method

hvap	79.50	kJ/mol	NIST Webbook
log10ws	-0.54		Aqueous Solubility Prediction Method
logp	1.166		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
ripol	2667.00		NIST Webbook
ripol	2667.00		NIST Webbook
tb	517.20	K	NIST Webbook
tb	516.35	K	NIST Webbook
tb	516.25 ± 1.00	K	NIST Webbook
tc	727.66	K	Joback Method
tf	271.56	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.58	J/mol×K	565.92	Joback Method
cpg	356.16	J/mol×K	592.88	Joback Method
cpg	366.31	J/mol×K	619.83	Joback Method
cpg	376.04	J/mol×K	646.79	Joback Method
cpg	385.36	J/mol×K	673.75	Joback Method
cpg	394.29	J/mol×K	700.71	Joback Method
cpg	402.84	J/mol×K	727.66	Joback Method
dvisc	0.2642980	Pa×s	271.56	Joback Method
dvisc	0.0200295	Pa×s	320.62	Joback Method
dvisc	0.0030104	Pa×s	369.68	Joback Method
dvisc	0.0007054	Pa×s	418.74	Joback Method
dvisc	0.0002241	Pa×s	467.80	Joback Method
dvisc	0.0000885	Pa×s	516.86	Joback Method
dvisc	0.0000411	Pa×s	565.92	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.63599e+01
Coeff. B	-5.07566e+03
Coeff. C	-8.49180e+01
Temperature range (K), min.	400.72
Temperature range (K), max.	544.32

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94962&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume