1,3-Octanediol

Other names:	Propane-1,3-diol, 1-pentyl- octane-1,3-diol
Inchi:	InChI=1S/C8H18O2/c1-2-3-4-5-8(10)6-7-9/h8-10H,2-7H2,1H3
InchiKey:	DCTMXCOHGKSXIZ-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CCCCCC(O)CCO
Mol. weight [g/mol]:	146.23
CAS:	23433-05-8

Physical Properties

Property code	Value	Unit	Source
gf	-259.60	kJ/mol	Joback Method
hf	-518.19	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.310		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1275.00		NIST Webbook
tb	566.36	K	Joback Method
tc	725.59	K	Joback Method
tf	286.56	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.21	J/mol×K	566.36	Joback Method
cpg	355.57	J/mol×K	592.90	Joback Method
cpg	365.52	J/mol×K	619.44	Joback Method
cpg	375.08	J/mol×K	645.97	Joback Method
cpg	384.24	J/mol×K	672.51	Joback Method
cpg	393.03	J/mol×K	699.05	Joback Method

cpg	401.45	J/mol×K	725.59	Joback Method
dvisc	0.1095688	Pa×s	286.56	Joback Method
dvisc	0.0119272	Pa×s	333.19	Joback Method
dvisc	0.0022382	Pa×s	379.83	Joback Method
dvisc	0.0006056	Pa×s	426.46	Joback Method
dvisc	0.0002120	Pa×s	473.09	Joback Method
dvisc	0.0000896	Pa×s	519.73	Joback Method
dvisc	0.0000436	Pa×s	566.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.85814e+01
Coeff. B	-5.95865e+03
Coeff. C	-9.02000e+01
Temperature range (K), min.	415.92
Temperature range (K), max.	539.24

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=C23433058&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume