1,2,6-Hexanetriol

Other names:	1,2,6-Trihydroxyhexane
	Hexane-1,2,6-triol
	Hexanetriol-(1,2,6)
Inchi:	InChI=1S/C6H14O3/c7-4-2-1-3-6(9)5-8/h6-9H,1-5H2
InchiKey:	ZWVMLYRJXORSEP-UHFFFAOYSA-N
Formula:	C6H14O3
SMILES:	OCCCCC(O)CO
Mol. weight [g/mol]:	134.17
CAS:	106-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-413.26	kJ/mol	Joback Method
hf	-629.14	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	78.60	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	-0.498		Crippen Method
mcvol	113.010	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
tb	612.78	K	Joback Method
tc	771.26	K	Joback Method
tf	305.95	K	NIST Webbook
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.79	J/mol×K	612.78	Joback Method
cpg	308.43	J/mol×K	639.19	Joback Method
cpg	315.76	J/mol×K	665.61	Joback Method
cpg	322.78	J/mol×K	692.02	Joback Method
cpg	329.51	J/mol×K	718.43	Joback Method
cpg	335.95	J/mol×K	744.85	Joback Method

cpg	342.12	J/mol×K	771.26	Joback Method
dvisc	0.0750496	Pa×s	324.84	Joback Method
dvisc	0.0067674	Pa×s	372.83	Joback Method
dvisc	0.0010564	Pa×s	420.82	Joback Method
dvisc	0.0002412	Pa×s	468.81	Joback Method
dvisc	0.0000724	Pa×s	516.80	Joback Method
dvisc	0.0000267	Pa×s	564.79	Joback Method
dvisc	0.0000115	Pa×s	612.78	Joback Method
hvapt	97.20	kJ/mol	413.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.20	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64932e+01
Coeff. B	-2.89503e+03
Coeff. C	-2.16650e+02
Temperature range (K), min.	395.29
Temperature range (K), max.	475.56

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C106694&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
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