

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:	ZWVMLYRJORSEP-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	342.12	J/molxK	771.26	Joback Method
cpg	335.95	J/molxK	744.85	Joback Method
cpg	329.51	J/molxK	718.43	Joback Method
cpg	322.78	J/molxK	692.02	Joback Method
cpg	315.76	J/molxK	665.61	Joback Method
cpg	308.43	J/molxK	639.19	Joback Method

cpg	300.79	J/molxK	612.78	Joback Method
dvisc	0.0750496	Paxs	324.84	Joback Method
dvisc	0.0000115	Paxs	612.78	Joback Method
dvisc	0.0000267	Paxs	564.79	Joback Method
dvisc	0.0000724	Paxs	516.80	Joback Method
dvisc	0.0002412	Paxs	468.81	Joback Method
dvisc	0.0010564	Paxs	420.82	Joback Method
dvisc	0.0067674	Paxs	372.83	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	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C106694&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
mccvol:	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

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