1,3-Hexanediol

Inchi: InChI=1S/C6H14O2/c1-2-3-6(8)4-5-7/h6-8H,2-5H2,1H3
InchiKey: AVIYEYCFMVPYST-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCCC(O)CCO
Mol. weight [g/mol]: 118.17
CAS: 21531-91-9

Physical Properties

Property code	Value	Unit	Source
gf	-276.44	kJ/mol	Joback Method
hf	-476.91	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.530		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
tb	520.60	K	Joback Method
tc	680.76	K	Joback Method
tf	264.02	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.37	J/mol×K	520.60	Joback Method
cpg	295.34	J/mol×K	654.07	Joback Method
cpg	287.99	J/mol×K	627.37	Joback Method
cpg	280.32	J/mol×K	600.68	Joback Method
cpg	272.33	J/mol×K	573.99	Joback Method
cpg	264.02	J/mol×K	547.29	Joback Method
cpg	302.40	J/mol×K	680.76	Joback Method

dvisc	0.0000740	Pa×s	520.60	Joback Method
dvisc	0.0001564	Pa×s	477.84	Joback Method
dvisc	0.0003828	Pa×s	435.07	Joback Method
dvisc	0.0011391	Pa×s	392.31	Joback Method
dvisc	0.0044260	Pa×s	349.55	Joback Method
dvisc	0.0251069	Pa×s	306.78	Joback Method
dvisc	0.2498961	Pa×s	264.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.79147e+01
Coeff. B	-5.48388e+03
Coeff. C	-8.24160e+01
Temperature range (K), min.	393.52
Temperature range (K), max.	517.53

Sources

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=C21531919&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

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