

2,3-Hexanediol

Inchi:	InChI=1S/C6H14O2/c1-3-4-6(8)5(2)7/h5-8H,3-4H2,1-2H3
InchiKey:	QCIYAEYRVFUFAP-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CCCC(O)C(C)O
Mol. weight [g/mol]:	118.17
CAS:	617-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-278.88	kJ/mol	Joback Method
hf	-482.19	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	906.00		NIST Webbook
ripol	1663.00		NIST Webbook
tb	478.15 ± 4.00	K	NIST Webbook
tc	683.21	K	Joback Method
tf	249.02	K	Joback Method
vc	0.398	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.68	J/mol×K	520.16	Joback Method
cpg	264.55	J/mol×K	547.34	Joback Method
cpg	273.06	J/mol×K	574.51	Joback Method
cpg	281.23	J/mol×K	601.69	Joback Method
cpg	289.05	J/mol×K	628.86	Joback Method
cpg	296.56	J/mol×K	656.04	Joback Method
cpg	303.74	J/mol×K	683.21	Joback Method

dvisc	0.6867154	Paxs	249.02	Joback Method
dvisc	0.0457867	Paxs	294.21	Joback Method
dvisc	0.0062787	Paxs	339.40	Joback Method
dvisc	0.0013734	Paxs	384.59	Joback Method
dvisc	0.0004135	Paxs	429.78	Joback Method
dvisc	0.0001565	Paxs	474.97	Joback Method
dvisc	0.0000701	Paxs	520.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48274e+01
Coeff. B	-4.29570e+03
Coeff. C	-7.40760e+01
Temperature range (K), min.	333.15
Temperature range (K), max.	525.50

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=C617301&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/ci9903071
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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