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	m3/kmol	Joback Method

Temperature Dependent Properties

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

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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=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/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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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