1,3-Pentanediol, 2-methyl-

Other names: 2-Methyl-1,3-pentanediol
Inchi: InChI=1S/C6H14O2/c1-3-6(8)5(2)4-7/h5-8H,3-4H2,1-2H3
InchiKey: SPXWGAHNKXLXAP-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCC(O)C(C)CO
Mol. weight [g/mol]: 118.17
CAS: 149-31-5

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	-0.73		Crippen Method
logp	0.386		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1005.00		NIST Webbook
tb	520.16	K	Joback Method
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	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	Pa×s	249.02	Joback Method
dvisc	0.0457867	Pa×s	294.21	Joback Method
dvisc	0.0062787	Pa×s	339.40	Joback Method
dvisc	0.0013734	Pa×s	384.59	Joback Method
dvisc	0.0004135	Pa×s	429.78	Joback Method
dvisc	0.0001565	Pa×s	474.97	Joback Method
dvisc	0.0000701	Pa×s	520.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62382e+01
Coeff. B	-4.83991e+03
Coeff. C	-7.83290e+01
Temperature range (K), min.	381.76
Temperature range (K), max.	521.27

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=C149315&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume