2,5-Hexanediol, 2,5-dimethyl-

Other names: 1,1,4,4-Tetramethyl-1,4-butanediol
2,5-Dimethyl-2,5-hexanediol
2,5-Dimethylhexane-2,5-diol
Inchi: InChI=1S/C8H18O2/c1-7(2,9)5-6-8(3,4)10/h9-10H,5-6H2,1-4H3
InchiKey: ZWNMRZQYWRLGMM-UHFFFAOYSA-N
Formula: C8H18O2
SMILES: CC(C)(O)CCC(C)(C)O
Mol. weight [g/mol]: 146.23
CAS: 110-03-2

Physical Properties

Property code	Value	Unit	Source
chs	-5039.00 ± 1.00	kJ/mol	NIST Webbook
gf	-251.48	kJ/mol	Joback Method
hf	-530.41	kJ/mol	Joback Method
hfs	-682.00 ± 1.00	kJ/mol	NIST Webbook
hfus	9.82	kJ/mol	Joback Method
hvap	85.20 ± 3.50	kJ/mol	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.308		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
tb	487.20	K	NIST Webbook
tc	732.08	K	Joback Method
tf	362.00 ± 3.00	K	NIST Webbook
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.29	J/mol×K	732.08	Joback Method
cpg	351.75	J/mol×K	560.34	Joback Method

cpg	362.94	J/mol×K	588.96	Joback Method
cpg	373.51	J/mol×K	617.59	Joback Method
cpg	383.50	J/mol×K	646.21	Joback Method
cpg	392.93	J/mol×K	674.83	Joback Method
cpg	401.85	J/mol×K	703.45	Joback Method
dvisc	0.0000412	Pa×s	560.34	Joback Method
dvisc	0.0655747	Pa×s	306.40	Joback Method
dvisc	0.0091067	Pa×s	348.72	Joback Method
dvisc	0.0019390	Pa×s	391.05	Joback Method
dvisc	0.0005585	Pa×s	433.37	Joback Method
dvisc	0.0002007	Pa×s	475.69	Joback Method
dvisc	0.0000853	Pa×s	518.02	Joback Method
hvapt	85.20	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63837e+01
Coeff. B	-4.83112e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	361.65
Temperature range (K), max.	512.91

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography: https://www.doi.org/10.1021/je060333x

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=C110032&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
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