

1,5-Pentanediol, 3-methyl-

Other names:	1,5-Dihydroxy-3-methylpentane 3-Methyl-1,5-pentanediol 3-methylpentane-1,5-diol
Inchi:	InChI=1S/C6H14O2/c1-6(2-4-7)3-5-8/h6-8H,2-5H2,1H3
InchiKey:	SXFJDZSJHVPHPH-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(CCO)CCO
Mol. weight [g/mol]:	118.17
CAS:	4457-71-0

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	-0.62		Crippen Method
logp	0.387		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
tb	520.60	K	Joback Method
tc	680.76	K	Joback Method
tf	264.02	K	Joback Method
vc	0.404	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

cpg	280.32	J/mol×K	600.68	Joback Method
cpg	287.99	J/mol×K	627.37	Joback Method
cpg	295.34	J/mol×K	654.07	Joback Method
dvisc	0.0000740	Paxs	520.60	Joback Method
dvisc	0.2498961	Paxs	264.02	Joback Method
dvisc	0.0251069	Paxs	306.78	Joback Method
dvisc	0.0044260	Paxs	349.55	Joback Method
dvisc	0.0011391	Paxs	392.31	Joback Method
dvisc	0.0003828	Paxs	435.07	Joback Method
dvisc	0.0001564	Paxs	477.84	Joback Method
hvapt	76.90	kJ/mol	443.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.98222e+01
Coeff. B	-6.21393e+03
Coeff. C	-8.61410e+01
Temperature range (K), min.	404.24
Temperature range (K), max.	514.37

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4457710&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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