

2,4-Pentanediol, 3-methyl-

Other names:	3-Methyl-2,4-pentanediol 3-Methylpentanediol-2,4 3-methylpentane-2,4-diol
Inchi:	InChI=1S/C6H14O2/c1-4(5(2)7)6(3)8/h4-8H,1-3H3
InchiKey:	RBQLGIKHSXQZTB-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(O)C(C)C(C)O
Mol. weight [g/mol]:	118.17
CAS:	5683-44-3

Physical Properties

Property code	Value	Unit	Source
gf	-281.32	kJ/mol	Joback Method
hf	-487.47	kJ/mol	Joback Method
hfus	8.90	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.384		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	963.00		NIST Webbook
tb	519.72	K	Joback Method
tc	685.78	K	Joback Method
tf	234.02	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.00	J/mol×K	519.72	Joback Method
cpg	265.09	J/mol×K	547.40	Joback Method
cpg	273.80	J/mol×K	575.07	Joback Method
cpg	282.15	J/mol×K	602.75	Joback Method
cpg	290.15	J/mol×K	630.43	Joback Method

cpg	297.80	J/mol×K	658.10	Joback Method
cpg	305.12	J/mol×K	685.78	Joback Method
dvisc	2.1854148	Pa×s	234.02	Joback Method
dvisc	0.0891622	Pa×s	281.64	Joback Method
dvisc	0.0091767	Pa×s	329.25	Joback Method
dvisc	0.0016777	Pa×s	376.87	Joback Method
dvisc	0.0004491	Pa×s	424.49	Joback Method
dvisc	0.0001568	Pa×s	472.10	Joback Method
dvisc	0.0000664	Pa×s	519.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53916e+01
Coeff. B	-4.51365e+03
Coeff. C	-7.58830e+01
Temperature range (K), min.	374.72
Temperature range (K), max.	523.66

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=C5683443&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

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