2,2-Dimethyl-1,3-butanediol

Other names: 1,3-Butanediol, 2,2-dimethyl-
Inchi: InChI=1S/C6H14O2/c1-5(8)6(2,3)4-7/h5,7-8H,4H2,1-3H3
InchiKey: QXKKYNIWAYERHT-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CC(O)C(C)(C)CO
Mol. weight [g/mol]: 118.17
CAS: 76-35-7

Physical Properties

Property code	Value	Unit	Source
gf	-273.60	kJ/mol	Joback Method
hf	-485.66	kJ/mol	Joback Method
hfus	8.53	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.386		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	517.37	K	Joback Method
tc	685.89	K	Joback Method
tf	266.44	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.90	J/mol×K	517.37	Joback Method
cpg	268.16	J/mol×K	545.46	Joback Method
cpg	276.95	J/mol×K	573.54	Joback Method
cpg	285.31	J/mol×K	601.63	Joback Method
cpg	293.24	J/mol×K	629.72	Joback Method
cpg	300.78	J/mol×K	657.80	Joback Method
cpg	307.94	J/mol×K	685.89	Joback Method
dvisc	0.3110979	Pa×s	266.44	Joback Method

dvisc	0.0300065	Pa×s	308.26	Joback Method
dvisc	0.0050606	Pa×s	350.08	Joback Method
dvisc	0.0012479	Pa×s	391.90	Joback Method
dvisc	0.0004031	Pa×s	433.73	Joback Method
dvisc	0.0001588	Pa×s	475.55	Joback Method
dvisc	0.0000728	Pa×s	517.37	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46146e+01
Coeff. B	-4.21339e+03
Coeff. C	-7.33530e+01
Temperature range (K), min.	367.44
Temperature range (K), max.	526.25

Sources

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=C76357&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

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

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