1,3-Butanediol, 2-methyl-

Other names: 2-Methyl-1,3-butanediol
2-Methylbutanediol-1,3
Inchi: InChI=1S/C5H12O2/c1-4(3-6)5(2)7/h4-7H,3H2,1-2H3
InchiKey: GNBPEYCZELNJMS-UHFFFAOYSA-N
Formula: C5H12O2
SMILES: CC(O)C(C)CO
Mol. weight [g/mol]: 104.15
CAS: 684-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-287.30	kJ/mol	Joback Method
hf	-461.55	kJ/mol	Joback Method
hfus	9.84	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.004		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	497.28	K	Joback Method
tc	661.20	K	Joback Method
tf	237.75	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.38	J/mol×K	661.20	Joback Method
cpg	213.59	J/mol×K	497.28	Joback Method
cpg	221.48	J/mol×K	524.60	Joback Method
cpg	229.06	J/mol×K	551.92	Joback Method
cpg	236.33	J/mol×K	579.24	Joback Method
cpg	243.30	J/mol×K	606.56	Joback Method
cpg	249.98	J/mol×K	633.88	Joback Method

dvisc	0.0000920	Pa×s	497.28	Joback Method
dvisc	1.1462269	Pa×s	237.75	Joback Method
dvisc	0.0710068	Pa×s	281.00	Joback Method
dvisc	0.0092386	Pa×s	324.26	Joback Method
dvisc	0.0019427	Pa×s	367.51	Joback Method
dvisc	0.0005673	Pa×s	410.77	Joback Method
dvisc	0.0002095	Pa×s	454.02	Joback Method
hvapt	62.40	kJ/mol	480.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54693e+01
Coeff. B	-4.44571e+03
Coeff. C	-7.26860e+01
Temperature range (K), min.	365.52
Temperature range (K), max.	510.35

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C684844&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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