2,3-Butanediol, 2,3-dimethyl-

Other names:	1,1,2,2-tetramethylethylene glycol 2,3-Dihydroxy-2,3-dimethylbutane 2,3-Dimethyl-2,3-butanediol 2,3-Dimethyl-2,3-dihydroxybutane Pinacol Tetramethylethylene glycol meso-2,3-Dimethyl-2,3-butanediol pinacone
Inchi:	InChI=1S/C6H14O2/c1-5(2,7)6(3,4)8/h7-8H,1-4H3
InchiKey:	IVDFJHOHABJVEH-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(C)(O)C(C)(C)O
Mol. weight [g/mol]:	118.17
CAS:	76-09-5

Physical Properties

Property code	Value	Unit	Source
gf	-268.32	kJ/mol	Joback Method
hf	-540.40 ± 9.40	kJ/mol	NIST Webbook
hfl	-606.30 ± 8.40	kJ/mol	NIST Webbook
hfus	4.64	kJ/mol	Joback Method
hvap	65.90	kJ/mol	NIST Webbook
hvap	65.90 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.08		Crippen Method
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	843.00		NIST Webbook
rinpol	850.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1338.00		NIST Webbook
tb	514.58	K	Joback Method
tc	689.00	K	Joback Method
tf	314.25 ± 1.00	K	NIST Webbook
tf	316.48 ± 0.05	K	NIST Webbook
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.50	J/mol×K	630.86	Joback Method
cpg	312.19	J/mol×K	689.00	Joback Method
cpg	305.06	J/mol×K	659.93	Joback Method
cpg	262.10	J/mol×K	514.58	Joback Method
cpg	271.78	J/mol×K	543.65	Joback Method
cpg	280.89	J/mol×K	572.72	Joback Method
cpg	289.45	J/mol×K	601.79	Joback Method
dvisc	0.0000759	Pa×s	514.58	Joback Method
dvisc	0.0003903	Pa×s	437.67	Joback Method
dvisc	0.0001611	Pa×s	476.13	Joback Method
dvisc	0.1478777	Pa×s	283.86	Joback Method
dvisc	0.0197037	Pa×s	322.31	Joback Method
dvisc	0.0040346	Pa×s	360.77	Joback Method
dvisc	0.0011213	Pa×s	399.22	Joback Method
hfust	14.70	kJ/mol	316.20	NIST Webbook
hfust	14.70	kJ/mol	316.20	NIST Webbook
hvapt	59.10	kJ/mol	397.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.70	K	98.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60845e+01
Coeff. B	-4.40158e+03
Coeff. C	-6.51240e+01

Temperature range (K), min.	314.25
Temperature range (K), max.	473.70

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76095&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
Concentration dependent melting enthalpy, crystallization velocity, and thermal cycling stability of pinacone hexahydrate:	https://www.doi.org/10.1016/j.tca.2018.10.025
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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