meso-2,3-butanediol

Other names:	(R,S)-Butan-2,3-diol
	2,3-Butanediol (erythro-)
	2,3-butanediol (erythro)
	2,3-butanediol (meso)
	erythro-2,3-Butanediol
	meso-butane-2,3-diol
Inchi:	InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3/t3-,4+
InchiKey:	OWBTYPJTUOEWEK-ZXZARUISSA-N
Formula:	C4H10O2
SMILES:	CC(O)C(C)O
Mol. weight [g/mol]:	90.12
CAS:	5341-95-7

Physical Properties

Property code	Value	Unit	Source
gf	-295.72	kJ/mol	Joback Method
hf	-440.91	kJ/mol	Joback Method
hfus	7.25	kJ/mol	Joback Method
hvap	66.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-0.25		Crippen Method
logp	-0.252		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
rinpol	743.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	759.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1546.00		NIST Webbook

ripol	1582.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1525.00		NIST Webbook
tb	457.00 ± 4.00	K	NIST Webbook
tb	456.70	K	NIST Webbook
tc	639.26	K	Joback Method
tf	307.65 ± 0.20	K	NIST Webbook
tf	308.15 ± 4.00	K	NIST Webbook
tf	306.65 ± 1.50	K	NIST Webbook
tf	307.55 ± 1.00	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.02	J/mol×K	611.78	Joback Method
cpg	199.24	J/mol×K	584.30	Joback Method
cpg	193.21	J/mol×K	556.83	Joback Method
cpg	186.92	J/mol×K	529.35	Joback Method
cpg	180.37	J/mol×K	501.88	Joback Method
cpg	173.55	J/mol×K	474.40	Joback Method
cpg	210.57	J/mol×K	639.26	Joback Method
dvisc	1.9625358	Pa×s	226.48	Joback Method
dvisc	0.0001208	Pa×s	474.40	Joback Method
dvisc	0.0002812	Pa×s	433.08	Joback Method
dvisc	0.0007824	Pa×s	391.76	Joback Method

dvisc	0.0027712	Pa×s	350.44	Joback Method
dvisc	0.0137635	Pa×s	309.12	Joback Method
dvisc	0.1120965	Pa×s	267.80	Joback Method
hfust	10.80	kJ/mol	306.60	NIST Webbook
hvapt	54.60	kJ/mol	433.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47795e+01
Coeff. B	-4.08372e+03
Coeff. C	-6.68060e+01
Temperature range (K), min.	348.60
Temperature range (K), max.	498.12

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5341957&Units=SI

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

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