DL-2,3-Butanediol

Other names: 2,3-Butanediol (DL)
2,3-Butanediol, (R*,R*)-(.+/-.)-
DL-2,3-Butandiol
Inchi: InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3
InchiKey: OWBTYPJTUOEWEK-UHFFFAOYSA-N
Formula: C4H10O2
SMILES: CC(O)C(C)O
Mol. weight [g/mol]: 90.12
CAS: 6982-25-8

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	57.08	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	-0.252		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
rinpol	747.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	793.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1620.00		NIST Webbook
tb	455.65 ± 0.70	K	NIST Webbook
tc	639.26	K	Joback Method
tf	280.75 ± 1.50	K	NIST Webbook
tf	279.65 ± 1.50	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.55	J/mol×K	474.40	Joback Method
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	210.57	J/mol×K	639.26	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
dvisc	1.9625358	Pa×s	226.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62156e+01
Coeff. B	-4.50380e+03
Coeff. C	-6.73200e+01
Temperature range (K), min.	350.08
Temperature range (K), max.	480.36

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=C6982258&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume