1,3-Propanediol, 2-butyl-2-ethyl-

Other names:	2-Butyl-2-ethyl-1,3-propanediol
	2-Butyl-2-ethylpropanediol
	2-Ethyl-2-Butylpropanediol-1,3
	2-Ethyl-2-butyl-1,3-propandeiol
	2-Ethyl-2-butyl-1,3-propanediol
	2-n-Butyl-2-ethyl-1,3-propanediol
	3,3-Bis(hydroxymethyl)heptane
	BEP
	NSC 406603
Inchi:	InChI=1S/C9H20O2/c1-3-5-6-9(4-2,7-10)8-11/h10-11H,3-8H2,1-2H3
InchiKey:	DSKYSDCYIODJPC-UHFFFAOYSA-N
Formula:	C9H20O2
SMILES:	CCCCC(CC)(CO)CO
Mol. weight [g/mol]:	160.25
CAS:	115-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-245.90	kJ/mol	Joback Method
hf	-542.30	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.558		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	586.45	K	Joback Method
tc	749.73	K	Joback Method
tf	314.25 ± 1.00	K	NIST Webbook
tf	314.80 ± 0.50	K	NIST Webbook
tf	312.20 ± 2.00	K	NIST Webbook
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.07	J/mol×K	695.31	Joback Method
cpg	456.42	J/mol×K	749.73	Joback Method
cpg	447.46	J/mol×K	722.52	Joback Method
cpg	395.74	J/mol×K	586.45	Joback Method
cpg	407.08	J/mol×K	613.66	Joback Method
cpg	417.91	J/mol×K	640.88	Joback Method
cpg	428.23	J/mol×K	668.09	Joback Method
dvisc	0.0001489	Pa×s	496.05	Joback Method
dvisc	0.0000660	Pa×s	541.25	Joback Method
dvisc	0.0000331	Pa×s	586.45	Joback Method
dvisc	0.0399974	Pa×s	315.25	Joback Method
dvisc	0.0058389	Pa×s	360.45	Joback Method
dvisc	0.0013088	Pa×s	405.65	Joback Method
dvisc	0.0003959	Pa×s	450.85	Joback Method
hfust	20.80	kJ/mol	317.30	NIST Webbook
hvapt	61.40 ± 0.60	kJ/mol	473.50	NIST Webbook
hvapt	67.20 ± 0.30	kJ/mol	473.50	NIST Webbook
hvapt	74.30 ± 0.30	kJ/mol	473.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.20	K	6.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72189e+01
Coeff. B	-5.50601e+03
Coeff. C	-8.99220e+01

Temperature range (K), min.	415.12
Temperature range (K), max.	552.33

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=C115844&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume