2,3-Butanediol, [R-(R*,R*)]-

Other names: [R,R]-2,3-butanediol
(R,R)-(-)-butane-2,3-diol
Inchi: InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3/t3-,4-/m0/s1
InchiKey: OWBTYPJTUOEWEK-IMJSIDKUSA-N
Formula: C4H10O2
SMILES: CC(O)C(C)O
Mol. weight [g/mol]: 90.12
CAS: 24347-58-8

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
ripol	1544.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1565.00		NIST Webbook
tb	474.40	K	Joback Method
tc	639.26	K	Joback Method
tf	226.48	K	Joback Method
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	180.37	J/mol×K	501.88	Joback Method
cpg	186.92	J/mol×K	529.35	Joback Method

cpg	193.21	J/mol×K	556.83	Joback Method
cpg	199.24	J/mol×K	584.30	Joback Method
cpg	205.02	J/mol×K	611.78	Joback Method
cpg	210.57	J/mol×K	639.26	Joback Method
dvisc	1.9625358	Pa×s	226.48	Joback Method
dvisc	0.1120965	Pa×s	267.80	Joback Method
dvisc	0.0137635	Pa×s	309.12	Joback Method
dvisc	0.0027712	Pa×s	350.44	Joback Method
dvisc	0.0007824	Pa×s	391.76	Joback Method
dvisc	0.0002812	Pa×s	433.08	Joback Method
dvisc	0.0001208	Pa×s	474.40	Joback Method
hvapt	52.60	kJ/mol	433.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.60	K	1.30	NIST Webbook

Sources

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=C24347588&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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