

2,3-Butanediol, (R,R)

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

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	743.00		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/molxK	474.40	Joback Method
cpg	180.37	J/molxK	501.88	Joback Method
cpg	186.92	J/molxK	529.35	Joback Method
cpg	193.21	J/molxK	556.83	Joback Method
cpg	199.24	J/molxK	584.30	Joback Method
cpg	205.02	J/molxK	611.78	Joback Method
cpg	210.57	J/molxK	639.26	Joback Method
dvisc	1.9625358	Paxs	226.48	Joback Method
dvisc	0.1120965	Paxs	267.80	Joback Method

dvisc	0.0137635	Paxs	309.12	Joback Method
dvisc	0.0027712	Paxs	350.44	Joback Method
dvisc	0.0007824	Paxs	391.76	Joback Method
dvisc	0.0002812	Paxs	433.08	Joback Method
dvisc	0.0001208	Paxs	474.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R635088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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