(E)-1,3-Butadien-1-ol

Other names: CH2=CHCH=CHOH (E)-
(E)-1-Hydroxy-1,3-butadiene
(1E)-1,3-Butadien-1-ol
(E)-1,3-Butadienol
Inchi: InChI=1S/C4H6O/c1-2-3-4-5/h2-5H,1H2/b4-3+
InchiKey: LNDKRVOOYMEYTC-ONEGZZNKSA-N
Formula: C4H6O
SMILES: C=CC=CO
Mol. weight [g/mol]: 70.09
CAS: 70411-98-2

Physical Properties

Property code	Value	Unit	Source
gf	14.04	kJ/mol	Joback Method
hf	-88.00 ± 5.00	kJ/mol	NIST Webbook
hfus	9.13	kJ/mol	Joback Method
hvap	40.47	kJ/mol	Joback Method
ie	8.51 ± 0.03	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	1.244		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4987.39	kPa	Joback Method
tb	383.94	K	Joback Method
tc	557.76	K	Joback Method
tf	188.82	K	Joback Method
vc	0.239	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.28	J/mol×K	383.94	Joback Method
cpg	111.28	J/mol×K	412.91	Joback Method
cpg	116.95	J/mol×K	441.88	Joback Method
cpg	122.32	J/mol×K	470.85	Joback Method

cpg	127.39	J/mol×K	499.82	Joback Method
cpg	132.19	J/mol×K	528.79	Joback Method
cpg	136.72	J/mol×K	557.76	Joback Method
dvisc	0.1354317	Pa×s	188.82	Joback Method
dvisc	0.0223091	Pa×s	221.34	Joback Method
dvisc	0.0058333	Pa×s	253.86	Joback Method
dvisc	0.0020685	Pa×s	286.38	Joback Method
dvisc	0.0009062	Pa×s	318.90	Joback Method
dvisc	0.0004625	Pa×s	351.42	Joback Method
dvisc	0.0002646	Pa×s	383.94	Joback Method

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=C70411982&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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