2,3-Butadien-1-ol

Inchi: InChI=1S/C4H6O/c1-2-3-4-5/h3,5H,1,4H2
InchiKey: JXKCVRNKAPHWJG-UHFFFAOYSA-N
Formula: C4H6O
SMILES: C=C=CCO
Mol. weight [g/mol]: 70.09
CAS: 18913-31-0

Physical Properties

Property code	Value	Unit	Source
gf	62.10	kJ/mol	Joback Method
hf	10.09	kJ/mol	Joback Method
hfus	11.05	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
ie	8.74	eV	NIST Webbook
ie	8.74	eV	NIST Webbook
log10ws	-0.49		Crippen Method
logp	0.320		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
rinpol	663.00		NIST Webbook
rinpol	663.00		NIST Webbook
tb	383.05	K	Joback Method
tc	558.99	K	Joback Method
tf	200.41	K	Joback Method
vc	0.239	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.14	J/mol×K	383.05	Joback Method
cpg	116.27	J/mol×K	412.37	Joback Method
cpg	121.24	J/mol×K	441.70	Joback Method
cpg	126.06	J/mol×K	471.02	Joback Method
cpg	130.73	J/mol×K	500.34	Joback Method

cpg	135.24	J/mol×K	529.67	Joback Method
cpg	139.60	J/mol×K	558.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.23936e+01
Coeff. B	-8.10714e+03
Coeff. C	-5.28090e+01
Temperature range (K), min.	305.32
Temperature range (K), max.	384.33

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18913310&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

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
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

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