3-Buten-2-ol, 3-methyl-

Other names:	2-Methyl-1-buten-3-ol
	3-Methyl-3-buten-2-ol
	CH2=C(CH3)CH(OH)CH3
	Methyl isopropenyl carbinol
Inchi:	InChI=1S/C5H10O/c1-4(2)5(3)6/h5-6H,1H2,2-3H3
InchiKey:	JEYLKNVLTAPJAF-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	C=C(C)C(C)O
Mol. weight [g/mol]:	86.13
CAS:	10473-14-0

Physical Properties

Property code	Value	Unit	Source
gf	-68.75	kJ/mol	Joback Method
hf	-188.40	kJ/mol	Joback Method
hfus	6.68	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
ie	9.61	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	0.943		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
rinpol	673.00		NIST Webbook
rinpol	737.00		NIST Webbook
tb	402.10	K	Joback Method
tc	573.89	K	Joback Method
tf	176.21	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.13	J/mol×K	402.10	Joback Method
cpg	163.23	J/mol×K	430.73	Joback Method

cpg	170.99	J/mol×K	459.36	Joback Method
cpg	178.42	J/mol×K	487.99	Joback Method
cpg	185.53	J/mol×K	516.62	Joback Method
cpg	192.33	J/mol×K	545.26	Joback Method
cpg	198.84	J/mol×K	573.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46215e+01
Coeff. B	-3.48916e+03
Coeff. C	-4.81800e+01
Temperature range (K), min.	287.34
Temperature range (K), max.	422.95

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10473140&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