3,3-Dimethylbutane-2-ol

Other names:	(CH3)3CCH(CH3)OH
	2,2-Dimethyl-3-butanol
	2-Butanol, 3,3-dimethyl-
	3,3-Dimethyl-2-butanol
	3,3-dimethylbutan-2-ol
	Pinacolyl alcohol
	Pinacolyl alcohol-tert-butyl methylcarbinol
	tert-Butyl Methyl carbinol
Inchi:	InChI=1S/C6H14O/c1-5(7)6(2,3)4/h5,7H,1-4H3
InchiKey:	DFOXKPDFWGNLJU-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CC(O)C(C)(C)C
Mol. weight [g/mol]:	102.17
CAS:	464-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-136.78	kJ/mol	Joback Method
hf	-333.43	kJ/mol	Joback Method
hfus	4.45	kJ/mol	Joback Method
hvap	53.80 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.62		Aqueous Solubility Prediction Method
log10ws	-0.62		Estimated Solubility Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	728.00		NIST Webbook
rinpol	740.60		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	722.30		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	723.40		NIST Webbook

ripol	1114.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1109.10		NIST Webbook
ripol	1114.00		NIST Webbook
tb	425.19	K	Joback Method
tc	600.02	K	Joback Method
tf	278.25	K	Aqueous Solubility Prediction Method
tt	278.40 ± 0.15	K	NIST Webbook
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.53	J/mol×K	570.88	Joback Method
cpg	267.98	J/mol×K	600.02	Joback Method
cpg	210.06	J/mol×K	425.19	Joback Method
cpg	220.98	J/mol×K	454.33	Joback Method
cpg	231.37	J/mol×K	483.47	Joback Method
cpg	241.24	J/mol×K	512.60	Joback Method
cpg	250.62	J/mol×K	541.74	Joback Method
dvisc	0.0002596	Pa×s	425.19	Joback Method
dvisc	0.0004905	Pa×s	388.60	Joback Method
dvisc	0.3533787	Pa×s	205.62	Joback Method
dvisc	0.0427885	Pa×s	242.22	Joback Method
dvisc	0.0090180	Pa×s	278.81	Joback Method
dvisc	0.0027278	Pa×s	315.40	Joback Method
dvisc	0.0010580	Pa×s	352.00	Joback Method
hvapt	46.80	kJ/mol	365.50	NIST Webbook
hvapt	48.30	kJ/mol	351.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.40014e+01
Coeff. B	-2.68958e+03
Coeff. C	-1.06359e+02
Temperature range (K), min.	278.45
Temperature range (K), max.	415.86

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C464073&Units=SI

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