1-Butanol, 3,3-dimethyl-

Other names: 3,3-Dimethyl-1-butanol
3,3-dimethylbutan-1-ol
Inchi: InChI=1S/C6H14O/c1-6(2,3)4-5-7/h7H,4-5H2,1-3H3
InchiKey: DUXCSEISVMREAX-UHFFFAOYSA-N
Formula: C6H14O
SMILES: CC(C)(C)CCO
Mol. weight [g/mol]: 102.17
CAS: 624-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-134.34	kJ/mol	Joback Method
hf	-328.15	kJ/mol	Joback Method
hfus	7.97	kJ/mol	Joback Method
hvap	58.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.50		Aqueous Solubility Prediction Method
log10ws	-0.50		Estimated Solubility Method
logp	1.415		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	779.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	816.70		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	815.50		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1249.00		NIST Webbook
tb	414.15 ± 2.00	K	NIST Webbook
tb	414.65 ± 2.00	K	NIST Webbook
tb	416.20	K	NIST Webbook
tb	415.65 ± 3.00	K	NIST Webbook
tb	412.15 ± 4.00	K	NIST Webbook
tb	416.00 ± 2.00	K	NIST Webbook

tb	414.15 ± 2.00	K	NIST Webbook
tb	416.15 ± 2.00	K	NIST Webbook
tb	414.15 ± 2.00	K	NIST Webbook
tb	414.65 ± 2.00	K	NIST Webbook
tc	596.64	K	Joback Method
tf	220.62	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.32	J/mol×K	511.13	Joback Method
cpg	230.71	J/mol×K	482.63	Joback Method
cpg	266.42	J/mol×K	596.64	Joback Method
cpg	258.15	J/mol×K	568.14	Joback Method
cpg	249.46	J/mol×K	539.64	Joback Method
cpg	210.01	J/mol×K	425.63	Joback Method
cpg	220.61	J/mol×K	454.13	Joback Method
cpl	236.08	J/mol×K	298.15	NIST Webbook
dvisc	0.0062994	Pa×s	288.96	Joback Method
dvisc	0.0022318	Pa×s	323.12	Joback Method
dvisc	0.0009643	Pa×s	357.29	Joback Method
dvisc	0.0004823	Pa×s	391.46	Joback Method
dvisc	0.0002697	Pa×s	425.63	Joback Method
dvisc	0.1316325	Pa×s	220.62	Joback Method
dvisc	0.0234865	Pa×s	254.79	Joback Method
hfust	9.54	kJ/mol	235.70	NIST Webbook
hvapt	49.40	kJ/mol	385.00	NIST Webbook
hvapt	50.80	kJ/mol	371.50	NIST Webbook
hvapt	52.40 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	55.40 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	58.60 ± 0.10	kJ/mol	328.00	NIST Webbook

Correlations

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

Coeff. A	1.83028e+01
Coeff. B	-4.46569e+03
Coeff. C	-6.83540e+01
Temperature range (K), min.	316.24
Temperature range (K), max.	412.10

Sources

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=C624953&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
vc:	Critical Volume