1-Butanol, 3-methyl-, benzoate

Other names:	1-(3-Methyl)butyl benzoate
	1-Butanol, 3-methyl-, 1-benzoate
	3-Methyl-1-butyl benzoate
	3-Methylbutyl benzoate
	Benzoic acid isoamyl ester
	Benzoic acid, 1-(3-methyl)butyl ester
	Benzoic acid, 3-methylbutyl ester
	Benzoic acid, isopentyl ester
	Isoamyl benzoate
	Isopentyl alcohol, benzoate
	Isopentyl benzoate
	NSC 9284
Inchi:	InChI=1S/C12H16O2/c1-10(2)8-9-14-12(13)11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey:	MLLAPOCBLWUFAP-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(C)CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	94-46-2

Physical Properties

Property code	Value	Unit	Source
gf	-73.79	kJ/mol	Joback Method
hf	-304.56	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.889		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1441.00		NIST Webbook

rinpol	1430.00	NIST Webbook
rinpol	1411.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1441.80	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1437.00	NIST Webbook
rinpol	1402.00	NIST Webbook
rinpol	1413.00	NIST Webbook
rinpol	1414.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1429.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1418.20	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1428.00	NIST Webbook
ripol	1930.00	NIST Webbook
ripol	1914.00	NIST Webbook
ripol	1895.00	NIST Webbook
ripol	1916.00	NIST Webbook
ripol	1929.00	NIST Webbook
ripol	1911.00	NIST Webbook
ripol	1913.00	NIST Webbook
ripol	1925.00	NIST Webbook
ripol	1944.00	NIST Webbook
ripol	1895.00	NIST Webbook
ripol	1891.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1904.00	NIST Webbook
ripol	1924.00	NIST Webbook
ripol	1937.00	NIST Webbook

ripol	1921.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1921.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1937.00		NIST Webbook
tb	535.50 ± 0.50	K	NIST Webbook
tb	535.15 ± 2.00	K	NIST Webbook
tc	786.80	K	Joback Method
tf	308.58	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.49	J/mol×K	751.74	Joback Method
cpg	451.37	J/mol×K	716.69	Joback Method
cpg	438.42	J/mol×K	681.64	Joback Method
cpg	424.63	J/mol×K	646.59	Joback Method
cpg	409.96	J/mol×K	611.54	Joback Method
cpg	394.41	J/mol×K	576.49	Joback Method
cpg	474.82	J/mol×K	786.80	Joback Method
dvisc	0.0029260	Pa×s	308.58	Joback Method
dvisc	0.0001725	Pa×s	576.49	Joback Method
dvisc	0.0002268	Pa×s	531.84	Joback Method
dvisc	0.0003136	Pa×s	487.19	Joback Method
dvisc	0.0004628	Pa×s	442.54	Joback Method
dvisc	0.0007455	Pa×s	397.88	Joback Method
dvisc	0.0013546	Pa×s	353.23	Joback Method
hvapt	51.60	kJ/mol	440.00	NIST Webbook
hvapt	56.00	kJ/mol	446.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.83771e+01
Coeff. B	-8.08880e+03
Coeff. C	5.27020e+01
Temperature range (K), min.	394.45
Temperature range (K), max.	566.39

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94462&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
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
vc:	Critical Volume

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