Butyl benzoate

Other names:	Anthrapole AZ
	Benzoic acid n-butyl ester
	Benzoic acid, butyl ester
	Butyl ester of benzoic acid
	Butylester kyseliny benzoove
	DAI CARI XBN
	Hipochem B-3-M
	Marvanol Carrier BB
	NSC 8474
	n-Butyl benzoate
Inchi:	InChI=1S/C11H14O2/c1-2-3-9-13-11(12)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3
InchiKey:	XSIFPSYPOVKYCO-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	136-60-7

Physical Properties

Property code	Value	Unit	Source
af	0.5800		KDB
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-3.48		Aqueous Solubility Prediction Method
logp	2.643		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	2600.00	kPa	KDB
pc	2400.00	kPa	Critical Point Measurements for n-Alkyl Benzoates (C8 to C13)
rinpol	1332.00		NIST Webbook
rinpol	1383.13		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1352.00		NIST Webbook

rinpol	1353.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1386.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1341.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1365.00	NIST Webbook
rinpol	1344.00	NIST Webbook
rinpol	1352.00	NIST Webbook
rinpol	1358.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1351.00	NIST Webbook
rinpol	1341.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1352.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1358.00	NIST Webbook
rinpol	1346.00	NIST Webbook
rinpol	1355.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1361.00	NIST Webbook
rinpol	1376.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1362.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1338.00	NIST Webbook
rinpol	1344.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1354.00	NIST Webbook
rinpol	1354.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1367.00	NIST Webbook
ripol	1882.00	NIST Webbook
ripol	1841.00	NIST Webbook
ripol	1871.00	NIST Webbook
ripol	1879.00	NIST Webbook
ripol	1901.00	NIST Webbook
ripol	1879.00	NIST Webbook

ripol	1884.00		NIST Webbook
ripol	1913.00		NIST Webbook
ripol	1841.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1841.00		NIST Webbook
ripol	1903.00		NIST Webbook
tb	523.45 ± 0.60	K	NIST Webbook
tb	521.50 ± 0.50	K	NIST Webbook
tb	522.20	K	NIST Webbook
tb	523.00	K	KDB
tb	522.15 ± 1.00	K	NIST Webbook
tc	723.00	K	KDB
tf	254.35	K	Aqueous Solubility Prediction Method
tf	250.75 ± 0.30	K	NIST Webbook
tf	251.00	K	KDB
vc	0.561	m3/kmol	KDB
zc	0.2426390		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.48	J/mol×K	623.81	Joback Method
cpg	421.37	J/mol×K	763.32	Joback Method
cpg	410.76	J/mol×K	728.44	Joback Method
cpg	399.42	J/mol×K	693.56	Joback Method
cpg	387.33	J/mol×K	658.68	Joback Method
cpg	346.39	J/mol×K	554.05	Joback Method
cpg	360.84	J/mol×K	588.93	Joback Method
dvisc	0.0012165	Pa×s	352.60	Joback Method
dvisc	0.0007317	Pa×s	392.89	Joback Method
dvisc	0.0004838	Pa×s	433.18	Joback Method
dvisc	0.0003432	Pa×s	473.47	Joback Method
dvisc	0.0002569	Pa×s	513.76	Joback Method
dvisc	0.0023060	Pa×s	312.31	Joback Method
dvisc	0.0002006	Pa×s	554.05	Joback Method

hvapt	57.10	kJ/mol	424.00	NIST Webbook
hvapt	58.10	kJ/mol	295.50	NIST Webbook
hvapt	54.40	kJ/mol	418.50	NIST Webbook
hvapt	60.40	kJ/mol	418.50	NIST Webbook
rhol	1006.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.83166e+01
Coeff. B	-9.10652e+03
Coeff. C	-5.84030e+00
Coeff. D	1.02964e-06
Temperature range (K), min.	251.65
Temperature range (K), max.	724.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1150.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136607&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1150
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical Point Measurements for n-Alkyl Benzoates (C8 to C13):	https://www.doi.org/10.1021/je700049s

Legend

af:	Acentric Factor
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
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
zc:	Critical Compressibility