Benzyl butyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester
	1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester
	1-Benzyl 2-butyl phthalate
	BBP
	Benzyl butyl phthalated
	Benzyl n-butyl phthalate
	Benzyl-butylester kyseliny ftalove
	Butyl benzyl phthalate
	Butyl phenylmethyl 1,2-benzenedicarboxylate
	NCI-C54375
	NSC 71001
	O1-butyl O2-(phenylmethyl) benzene-1,2-dicarboxylate
	Palatinol BB
	Phthalic acid, benzyl butyl ester
	Santicizer 160
	Santicizer S 160
	Sicol
	Sicol 160
	Spatozoate
	Unimoll BB
	benzyl butyl 1,2-benzenedioate
	n-Butyl benzyl phthalate
Inchi:	InChI=1S/C19H20O4/c1-2-3-13-22-18(20)16-11-7-8-12-17(16)19(21)23-14-15-9-5-4-6-10
InchiKey:	IRIAEXORFWYRCZ-UHFFFAOYSA-N
Formula:	C19H20O4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1
Mol. weight [g/mol]:	312.36
CAS:	85-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-143.55	kJ/mol	Joback Method
hf	-463.50	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-5.65		Aqueous Solubility Prediction Method

logp	4.000		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	378.40		NIST Webbook
rinpol	378.40		NIST Webbook
rinpol	2358.90		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	845.04	K	Joback Method
tc	1070.91	K	Joback Method
tf	513.57	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.43	J/mol×K	845.04	Joback Method
cpg	738.52	J/mol×K	882.69	Joback Method
cpg	751.35	J/mol×K	920.33	Joback Method
cpg	762.96	J/mol×K	957.98	Joback Method
cpg	773.37	J/mol×K	995.62	Joback Method
cpg	782.63	J/mol×K	1033.27	Joback Method
cpg	790.77	J/mol×K	1070.91	Joback Method
dvisc	0.0003309	Pa×s	568.81	Joback Method
dvisc	0.0005675	Pa×s	513.57	Joback Method
dvisc	0.0002123	Pa×s	624.06	Joback Method
dvisc	0.0001464	Pa×s	679.30	Joback Method
dvisc	0.0001068	Pa×s	734.55	Joback Method
dvisc	0.0000814	Pa×s	789.79	Joback Method
dvisc	0.0000643	Pa×s	845.04	Joback Method

hvapt	109.80	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure
hvapt	89.00	kJ/mol	466.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00444
Determination of Henry's Law Constant Using Diffusion in Air and Water:	https://www.doi.org/10.1021/je300954s
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume