Butylparaben

Other names:	4-(Butoxycarbonyl)phenol
	4-Hydroxybenzoic acid, butyl ester
	Aseptoform butyl
	Benzoic acid, 4-hydroxy-, butyl ester
	Benzoic acid, p-hydroxy-, butyl ester
	Butoben
	Butyl 4-hydroxybenzoate
	Butyl Butex
	Butyl Tegosept
	Butyl chemosept
	Butyl p-hydroxybenzoate
	Butyl parasept
	Lexgard B
	NSC 8475
	Nipabutyl
	Preserval B
	SPF
	Solbrol B
	Tegosept B
	Tegosept butyl
	butyl paraben
	n-Butyl p-hydroxybenzoate
	n-Butyl parahydroxybenzoate
	n-Butyl-4-hydroxybenzoate
	n-Butyl-paraben
	p-Hydroxybenzoic acid, butyl ester
	p-Hydroxybenzoic acid, n-butyl ester
Inchi:	InChI=1S/C11H14O3/c1-2-3-8-14-11(13)9-4-6-10(12)7-5-9/h4-7,12H,2-3,8H2,1H3
InchiKey:	QFOHBWFCKVYLES-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCCCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	194.23
CAS:	94-26-8

Physical Properties

Property code	Value	Unit	Source

gf	-234.39	kJ/mol	Joback Method
hf	-455.95	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Thermodynamics of molecular solids in organic solvents
hsub	108.40 ± 0.80	kJ/mol	NIST Webbook
hvap	64.53	kJ/mol	Joback Method
log10ws	-3.10		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.86		Aqueous Solubility Prediction Method
logp	2.349		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	634.67	K	Joback Method
tc	854.09	K	Joback Method
tf	342.20	K	Aqueous Solubility Prediction Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.78	J/mol×K	854.09	Joback Method
cpg	398.53	J/mol×K	634.67	Joback Method
cpg	411.37	J/mol×K	671.24	Joback Method
cpg	423.41	J/mol×K	707.81	Joback Method
cpg	434.71	J/mol×K	744.38	Joback Method
cpg	445.32	J/mol×K	780.95	Joback Method
cpg	455.33	J/mol×K	817.52	Joback Method
dvisc	0.0000257	Pa×s	634.67	Joback Method
dvisc	0.0007210	Pa×s	424.03	Joback Method
dvisc	0.0003344	Pa×s	459.14	Joback Method
dvisc	0.0001730	Pa×s	494.24	Joback Method
dvisc	0.0000977	Pa×s	529.35	Joback Method
dvisc	0.0000592	Pa×s	564.46	Joback Method
dvisc	0.0000380	Pa×s	599.56	Joback Method
hfust	26.60	kJ/mol	341.80	NIST Webbook

Sources

Phase equilibrium and mechanisms of crystallization in liquid-liquid phase separating system:	https://www.doi.org/10.1016/j.fluid.2014.11.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Butyl Paraben in Methanol, Ethanol, Propanol, Ethyl Acetate, Acetone, and Acetonitrile:	https://www.doi.org/10.1021/je1006289
Thermodynamics of molecular solids in organic solvents:	https://www.doi.org/10.1016/j.jct.2011.12.015
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Solubility of Parabens in Subcritical Water:	https://www.doi.org/10.1021/je4010883
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94268&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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