

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
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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
rropol	1671.00		NIST Webbook
rropol	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	455.33	J/mol×K	817.52	Joback Method
cpg	445.32	J/mol×K	780.95	Joback Method
cpg	434.71	J/mol×K	744.38	Joback Method
cpg	423.41	J/mol×K	707.81	Joback Method
cpg	411.37	J/mol×K	671.24	Joback Method
cpg	398.53	J/mol×K	634.67	Joback Method
dvisc	0.0007210	Paxs	424.03	Joback Method
dvisc	0.0000257	Paxs	634.67	Joback Method
dvisc	0.0000380	Paxs	599.56	Joback Method
dvisc	0.0000592	Paxs	564.46	Joback Method
dvisc	0.0000977	Paxs	529.35	Joback Method
dvisc	0.0001730	Paxs	494.24	Joback Method
dvisc	0.0003344	Paxs	459.14	Joback Method
hfust	26.60	kJ/mol	341.80	NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Thermodynamics of molecular solids in organic solvents:	https://www.doi.org/10.1016/j.jct.2011.12.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Solubility of Parabens in Subcritical Water:	https://www.doi.org/10.1021/je4010883
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Butyl Paraben in Methanol, Ethanol, Propanol, Ethyl Acetate, Phase equilibrium and mechanisms of crystallization in liquid-liquid phase separating system:	https://www.doi.org/10.1021/je1006289 https://www.doi.org/10.1016/j.fluid.2014.11.007

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

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