Benzoic acid, 2-hydroxy-, butyl ester

Other names:	Salicylic acid, butyl ester
	Butyl o-hydroxybenzoate
	Butyl salicylate
	n-Butyl salicylate
	n-Butyl o-hydroxybenzoate
	2-Hydroxy-benzoic acid, butyl ester
	Salicylic acid, n-butyl ester
	Butyl 2-hydroxybenzoate
	NSC 1511
	NSC 403676
Inchi:	InChI=1S/C11H14O3/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h4-7,12H,2-3,8H2,1H3
InchiKey:	YFDUWSBGVPBWKF-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCCCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	194.23
CAS:	2052-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-234.39	kJ/mol	Joback Method
hf	-455.95	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.349		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1454.80		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1454.80		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1457.00		NIST Webbook
ripol	1976.00		NIST Webbook
tb	544.20	K	NIST Webbook

tc	854.09	K	Joback Method
tf	424.03	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	464.78	J/mol×K	854.09	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
dvisc	0.0000257	Pa×s	634.67	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2052144&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume