Benzoic acid, 2-hydroxy-, 2-methylpropyl ester

Other names:	Salicylic acid, isobutyl ester
	Isobutyl o-hydroxybenzoate
	Isobutyl salicylate
	2-Isobutoxycarbonylphenol
	2-Methylpropyl o-hydroxybenzoate
	Orchindone
	2-Methylpropyl salicylate
	Salicylic acid, 2-methylpropyl ester
Inchi:	InChI=1S/C11H14O3/c1-8(2)7-14-11(13)9-5-3-4-6-10(9)12/h3-6,8,12H,7H2,1-2H3
InchiKey:	PTXDBYSCVQQBNF-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CC(C)COC(=O)c1ccccc1O
Mol. weight [g/mol]:	194.23
CAS:	87-19-4

Physical Properties

Property code	Value	Unit	Source
gf	-236.83	kJ/mol	Joback Method
hf	-461.23	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.205		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1398.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1896.00		NIST Webbook
tb	634.23	K	Joback Method
tc	858.14	K	Joback Method
tf	409.03	K	Joback Method

vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.03	J/mol×K	634.23	Joback Method
cpg	456.95	J/mol×K	820.82	Joback Method
cpg	446.79	J/mol×K	783.50	Joback Method
cpg	435.99	J/mol×K	746.18	Joback Method
cpg	424.47	J/mol×K	708.87	Joback Method
cpg	412.17	J/mol×K	671.55	Joback Method
cpg	466.52	J/mol×K	858.14	Joback Method
dvisc	0.0000240	Pa×s	634.23	Joback Method
dvisc	0.0000367	Pa×s	596.70	Joback Method
dvisc	0.0000595	Pa×s	559.16	Joback Method
dvisc	0.0001034	Pa×s	521.63	Joback Method
dvisc	0.0001960	Pa×s	484.10	Joback Method
dvisc	0.0004133	Pa×s	446.56	Joback Method
dvisc	0.0009998	Pa×s	409.03	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87194&Units=SI
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

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