Benzoic acid, 2-hydroxy-, 3-methyl-2-butenyl ester

Other names: 2-Buten-1-ol, 3-methyl-, salicylate
3-Methyl-2-butenyl salicylate
Prenyl salicylate

Inchi: InChI=1S/C12H14O3/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/h3-7,13H,8H2,1-2H3

InchiKey: MCAYDAOGSVHGEE-UHFFFAOYSA-N

Formula: C12H14O3

SMILES: CC(C)=CCOC(=O)c1ccccc1O

Mol. weight [g/mol]: 206.24

CAS: 68555-58-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.30	kJ/mol	Joback Method
hf	-369.16	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	66.79	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.515		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	661.59	K	Joback Method
tc	889.73	K	Joback Method
tf	416.26	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.51	J/mol×K	661.59	Joback Method
cpg	438.55	J/mol×K	699.61	Joback Method
cpg	450.74	J/mol×K	737.64	Joback Method
cpg	462.17	J/mol×K	775.66	Joback Method
cpg	472.93	J/mol×K	813.69	Joback Method
cpg	483.11	J/mol×K	851.71	Joback Method

cpg	492.80	J/mol×K	889.73	Joback Method

Sources

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=C68555588&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume