Benzoic acid, 2-hydroxy-, 2-propenyl ester

Other names:	Salicylic acid, allyl ester
	Allyl salicylate
Inchi:	InChI=1S/C10H10O3/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h2-6,11H,1,7H2
InchiKey:	YYKBLDCLPBWOOE-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	C=CCOC(=O)c1ccccc1O
Mol. weight [g/mol]:	178.18
CAS:	10484-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-154.97	kJ/mol	Joback Method
hf	-309.88	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	61.63	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.735		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	1339.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1946.00		NIST Webbook
tb	608.47	K	Joback Method
tc	836.63	K	Joback Method
tf	411.00	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.63	J/mol×K	608.47	Joback Method
cpg	340.98	J/mol×K	646.50	Joback Method
cpg	351.54	J/mol×K	684.52	Joback Method
cpg	361.38	J/mol×K	722.55	Joback Method

cpg	370.57	J/mol×K	760.58	Joback Method
cpg	379.18	J/mol×K	798.60	Joback Method
cpg	387.29	J/mol×K	836.63	Joback Method
dvisc	0.0008638	Pa×s	411.00	Joback Method
dvisc	0.0004122	Pa×s	443.91	Joback Method
dvisc	0.0002178	Pa×s	476.82	Joback Method
dvisc	0.0001250	Pa×s	509.74	Joback Method
dvisc	0.0000767	Pa×s	542.65	Joback Method
dvisc	0.0000498	Pa×s	575.56	Joback Method
dvisc	0.0000339	Pa×s	608.47	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=C10484090&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
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