

Benzaldehyde, 2-hydroxy-3-(2-propenyl)-

Other names:	Salicylaldehyde, 3-allyl- 3-Allylsalicylaldehyde
Inchi:	InChI=1S/C10H10O2/c1-2-4-8-5-3-6-9(7-11)10(8)12/h2-3,5-7,12H,1,4H2
InchiKey:	INLWEXRRMUMHKB-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	C=CCc1cccc(C=O)c1O
Mol. weight [g/mol]:	162.19
CAS:	24019-66-7

Physical Properties

Property code	Value	Unit	Source
gf	-30.20	kJ/mol	Joback Method
hf	-162.13	kJ/mol	Joback Method
hfus	22.10	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.933		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	585.82	K	Joback Method
tc	812.84	K	Joback Method
tf	393.36	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.24	J/mol×K	585.82	Joback Method
cpg	318.26	J/mol×K	623.66	Joback Method
cpg	328.49	J/mol×K	661.49	Joback Method
cpg	338.01	J/mol×K	699.33	Joback Method
cpg	346.90	J/mol×K	737.17	Joback Method
cpg	355.26	J/mol×K	775.00	Joback Method
cpg	363.16	J/mol×K	812.84	Joback Method

dvisc	0.0013062	Pa×s	393.36	Joback Method
dvisc	0.0006216	Pa×s	425.44	Joback Method
dvisc	0.0003282	Pa×s	457.51	Joback Method
dvisc	0.0001885	Pa×s	489.59	Joback Method
dvisc	0.0001159	Pa×s	521.67	Joback Method
dvisc	0.0000753	Pa×s	553.74	Joback Method
dvisc	0.0000514	Pa×s	585.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.00 ± 2.00	K	3.30	NIST Webbook

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=C24019667&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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