

2-Propenal, 3-(4-hydroxy-3,5-dimethoxyphenyl), (Z)-

Inchi:	InChI=1S/C11H12O4/c1-14-9-6-8(4-3-5-12)7-10(15-2)11(9)13/h3-7,13H,1-2H3/b4-3-
InchiKey:	CDICDSOGTRCHMG-ARJAWSKDSA-N
Formula:	C11H12O4
SMILES:	COc1cc(C=CC=O)cc(OC)c1O
Mol. weight [g/mol]:	208.21

Physical Properties

Property code	Value	Unit	Source
gf	-249.03	kJ/mol	Joback Method
hf	-466.89	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	68.19	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.621		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinsol	1856.00		NIST Webbook
tb	666.00	K	Joback Method
tc	888.57	K	Joback Method
tf	458.29	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.69	J/molxK	666.00	Joback Method
cpg	410.06	J/molxK	703.10	Joback Method
cpg	420.78	J/molxK	740.19	Joback Method
cpg	430.90	J/molxK	777.29	Joback Method
cpg	440.47	J/molxK	814.38	Joback Method
cpg	449.53	J/molxK	851.48	Joback Method
cpg	458.15	J/molxK	888.57	Joback Method
dvisc	0.0002831	Paxs	458.29	Joback Method
dvisc	0.0001487	Paxs	492.91	Joback Method

dvisc	0.0000850	Paxs	527.53	Joback Method
dvisc	0.0000520	Paxs	562.14	Joback Method
dvisc	0.0000337	Paxs	596.76	Joback Method
dvisc	0.0000229	Paxs	631.38	Joback Method
dvisc	0.0000162	Paxs	666.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R88425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

Latest version available from:

<https://www.chemeo.com/cid/64-583-4/2-Propenal-3-4-hydroxy-3-5-dimethoxyphenyl-Z.pdf>

Generated by Cheméo on 2024-07-21 17:24:36.147931023 +0000 UTC m=+272545.395036369.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.