

Phenol, 4-(1-propenyl)-2,6-dimethoxy, (Z)-

Inchi:	InChI=1S/C11H14O3/c1-4-5-8-6-9(13-2)11(12)10(7-8)14-3/h4-7,12H,1-3H3/b5-4-
InchiKey:	YFHOHYAUMDHSBX-PLNGDYQASA-N
Formula:	C11H14O3
SMILES:	CC=Cc1cc(OC)c(O)c(OC)c1
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
gf	-149.51	kJ/mol	Joback Method
hf	-381.31	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.442		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1604.00		NIST Webbook
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tb	617.34	K	Joback Method
tc	838.09	K	Joback Method
tf	416.29	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.89	J/molxK	617.34	Joback Method
cpg	442.79	J/molxK	801.30	Joback Method
cpg	432.43	J/molxK	764.51	Joback Method
cpg	421.52	J/molxK	727.71	Joback Method
cpg	409.99	J/molxK	690.92	Joback Method
cpg	397.79	J/molxK	654.13	Joback Method
cpg	452.62	J/molxK	838.09	Joback Method
dvisc	0.0000181	Paxs	617.34	Joback Method

dvisc	0.0000263	Paxs	583.83	Joback Method
dvisc	0.0000399	Paxs	550.32	Joback Method
dvisc	0.0000640	Paxs	516.82	Joback Method
dvisc	0.0001096	Paxs	483.31	Joback Method
dvisc	0.0002034	Paxs	449.80	Joback Method
dvisc	0.0004170	Paxs	416.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R88489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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