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

Other names:	Phenol, 4-allyl-2,6-dimethoxy-
	Methoxyeugenol
	2,6-Dimethoxy-4-allylphenol
	4-Allyl-2,6-dimethoxyphenol
	4-Hydroxy-3,5-dimethoxyallylbenzene
	2,6-Dimethoxy-4-(2-propenyl)phenol
	4-(2-Propenyl)-2,6-dimethoxyphenol (4-allylsyringol)
	4-Allyl-2,6-dimetoxyphenol
	4-Allylsyringol
	Phenol, 4-(2-propenyl)-2,6-dimethoxy
Inchi:	InChI=1S/C11H14O3/c1-4-5-8-6-9(13-2)11(12)10(7-8)14-3/h4,6-7,12H,1,5H2,2-3H3
InchiKey:	FWMPKHMKIJDEMJ-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	C=CCc1cc(OC)c(O)c(OC)c1
Mol. weight [g/mol]:	194.23
CAS:	6627-88-9

Physical Properties

Property code	Value	Unit	Source
gf	-141.89	kJ/mol	Joback Method
hf	-373.10	kJ/mol	Joback Method
hfus	24.39	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.138		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1606.50		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1546.00		NIST Webbook

rinpol	1558.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1606.50		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1615.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2544.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2543.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2543.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2563.00		NIST Webbook
tb	609.86	K	Joback Method
tc	825.91	K	Joback Method
tf	419.61	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.80	J/mol×K	609.86	Joback Method
cpg	442.43	J/mol×K	789.90	Joback Method
cpg	432.12	J/mol×K	753.90	Joback Method
cpg	421.25	J/mol×K	717.89	Joback Method
cpg	409.76	J/mol×K	681.88	Joback Method
cpg	397.62	J/mol×K	645.87	Joback Method
cpg	452.20	J/mol×K	825.91	Joback Method
dvisc	0.0000229	Pa×s	609.86	Joback Method
dvisc	0.0000327	Pa×s	578.15	Joback Method
dvisc	0.0000487	Pa×s	546.44	Joback Method
dvisc	0.0000762	Pa×s	514.74	Joback Method
dvisc	0.0001264	Pa×s	483.03	Joback Method

dvisc	0.0002251	Pa×s	451.32	Joback Method
dvisc	0.0004375	Pa×s	419.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.70	K	1.50	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=C6627889&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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