

4-ALLYLPHENOL

Other names:	4-(2-Propenyl)phenol 4-(Prop-2-enyl)-phenol 4-Allylphenol Chavicol Phenol, p-allyl- p-Allylphenol p-Chavicol p-Hydroxyallylbenzene «gamma»-(p-Hydroxyphenyl)-«alpha»-propylene
Inchi:	InChI=1S/C9H10O/c1-2-3-8-4-6-9(10)7-5-8/h2,4-7,10H,1,3H2
InchiKey:	RGIBXDHONMXTLI-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	C=CCc1ccc(O)cc1
Mol. weight [g/mol]:	134.18

Physical Properties

Property code	Value	Unit	Source
hf	-28.45	kJ/mol	Cheméo Relay (1.0)
hfus	17.61	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-1.54		Cheméo Relay (1.0)
logp	2.121		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1214.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	195.70		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1214.00		NIST Webbook

rinpol	1203.00	NIST Webbook
rinpol	1253.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1232.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1219.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1233.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1229.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1252.00	NIST Webbook
ripol	2316.00	NIST Webbook
ripol	2324.00	NIST Webbook
ripol	2338.00	NIST Webbook
ripol	2329.00	NIST Webbook
ripol	2300.00	NIST Webbook
ripol	2328.00	NIST Webbook
ripol	2358.00	NIST Webbook
ripol	2282.00	NIST Webbook
ripol	2342.00	NIST Webbook
ripol	2345.00	NIST Webbook
ripol	2345.00	NIST Webbook
ripol	2338.00	NIST Webbook
ripol	2320.00	NIST Webbook
ripol	2346.00	NIST Webbook
ripol	2329.00	NIST Webbook
ripol	2329.00	NIST Webbook
ripol	2339.00	NIST Webbook
ripol	2358.00	NIST Webbook
ripol	2327.00	NIST Webbook

ripol	2340.00		NIST Webbook
tb	511.76	K	Cheméo Relay (1.0)
tc	723.88	K	Cheméo Relay (1.0)
tf	308.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.21	J/mol×K	509.30	Joback Method
cpg	261.41	J/mol×K	547.17	Joback Method
cpg	272.66	J/mol×K	585.04	Joback Method
cpg	283.06	J/mol×K	622.91	Joback Method
cpg	292.68	J/mol×K	660.78	Joback Method
cpg	301.63	J/mol×K	698.65	Joback Method
cpg	309.98	J/mol×K	736.53	Joback Method
dvisc	0.0042028	Pa×s	327.57	Joback Method
dvisc	0.0016414	Pa×s	357.86	Joback Method
dvisc	0.0007423	Pa×s	388.15	Joback Method
dvisc	0.0003766	Pa×s	418.44	Joback Method
dvisc	0.0002094	Pa×s	448.72	Joback Method
dvisc	0.0001254	Pa×s	479.01	Joback Method
dvisc	0.0000798	Pa×s	509.30	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C501928&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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