

Phenol, 4-(2-propenyl)-, acetate

Other names:	4-Allylphenyl acetate Chavicol, acetate 4-(2-Propenyl)phenyl acetate
Inchi:	InChI=1S/C11H12O2/c1-3-4-10-5-7-11(8-6-10)13-9(2)12/h3,5-8H,1,4H2,2H3
InchiKey:	AXHHVVBUEOKYKJO-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	C=CCc1ccc(OC(C)=O)cc1
Mol. weight [g/mol]:	176.21
CAS:	61499-22-7

Physical Properties

Property code	Value	Unit	Source
gf	-1.56	kJ/mol	Joback Method
hf	-164.68	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.340		Crippen Method
mcpvol	145.230	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
ripol	1314.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1350.60		NIST Webbook
ripol	1350.60		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1949.00		NIST Webbook
tb	555.71	K	Joback Method
tc	770.47	K	Joback Method
tf	323.07	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.57	J/mol×K	555.71	Joback Method
cpg	340.05	J/mol×K	591.50	Joback Method
cpg	352.75	J/mol×K	627.30	Joback Method
cpg	364.71	J/mol×K	663.09	Joback Method
cpg	375.94	J/mol×K	698.88	Joback Method
cpg	386.46	J/mol×K	734.67	Joback Method
cpg	396.28	J/mol×K	770.47	Joback Method
dvisc	0.0016626	Pa×s	323.07	Joback Method
dvisc	0.0009678	Pa×s	361.84	Joback Method
dvisc	0.0006256	Pa×s	400.62	Joback Method
dvisc	0.0004367	Pa×s	439.39	Joback Method
dvisc	0.0003232	Pa×s	478.16	Joback Method
dvisc	0.0002502	Pa×s	516.94	Joback Method
dvisc	0.0002008	Pa×s	555.71	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=C61499227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/42-223-7/Phenol-4-2-propenyl-acetate.pdf>

Generated by Cheméo on 2025-12-06 04:42:16.710686877 +0000 UTC m=+4744334.240727540.

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