Phenol, 5-methyl-2-(1-methylethyl)-, acetate

Other names:	O-Acetylthymol
	Thymol acetate
	Thymyl acetate
	Thimyl acetate
Inchi:	InChI=1S/C12H16O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h5-8H,1-4H3
InchiKey:	WFMIUXMJJBBOGJ-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(=O)Oc1cc(C)ccc1C(C)C
Mol. weight [g/mol]:	192.25
CAS:	528-79-0

Physical Properties

Property code	Value	Unit	Source
gf	-93.05	kJ/mol	Joback Method
hf	-327.50	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	54.67	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.044		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1355.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1357.00		NIST Webbook

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rinpol	1358.00		NIST Webbook
rinpol	1352.00		NIST Webbook
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rinpol	1353.00		NIST Webbook
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rinpol	1345.00		NIST Webbook
rinpol	1351.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
tb	586.45	K	Joback Method
tc	798.75	K	Joback Method
tf	333.62	K	Joback Method

vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.82	J/mol×K	586.45	Joback Method
cpg	461.11	J/mol×K	763.37	Joback Method
cpg	449.20	J/mol×K	727.98	Joback Method
cpg	436.53	J/mol×K	692.60	Joback Method
cpg	423.09	J/mol×K	657.22	Joback Method
cpg	408.86	J/mol×K	621.83	Joback Method
cpg	472.25	J/mol×K	798.75	Joback Method
dvisc	0.0001653	Pa×s	586.45	Joback Method
dvisc	0.0002091	Pa×s	544.31	Joback Method
dvisc	0.0002750	Pa×s	502.17	Joback Method
dvisc	0.0003803	Pa×s	460.04	Joback Method
dvisc	0.0005614	Pa×s	417.90	Joback Method
dvisc	0.0009045	Pa×s	375.76	Joback Method
dvisc	0.0016439	Pa×s	333.62	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=C528790&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

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https://www.chemeo.com/cid/47-717-4/Phenol-5-methyl-2-1-methylethyl-acetate.pdf
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