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

Other names:	Carvacryl acetate
	5-Isopropyl-o-tolyl acetate
	Carvacrol acetate
Inchi:	InChI=1S/C12H16O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h5-8H,1-4H3
InchiKey:	OXZSUQJHKQOGOK-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(=O)Oc1cc(C(C)C)ccc1C
Mol. weight [g/mol]:	192.25
CAS:	6380-28-5

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	1368.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1341.00		NIST Webbook

rinpol	1376.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1362.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1868.00		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	408.86	J/mol×K	621.83	Joback Method
cpg	423.09	J/mol×K	657.22	Joback Method
cpg	436.53	J/mol×K	692.60	Joback Method
cpg	449.20	J/mol×K	727.98	Joback Method
cpg	461.11	J/mol×K	763.37	Joback Method
cpg	472.25	J/mol×K	798.75	Joback Method
dvisc	0.0016439	Pa×s	333.62	Joback Method
dvisc	0.0009045	Pa×s	375.76	Joback Method
dvisc	0.0005614	Pa×s	417.90	Joback Method
dvisc	0.0003803	Pa×s	460.04	Joback Method
dvisc	0.0002750	Pa×s	502.17	Joback Method
dvisc	0.0002091	Pa×s	544.31	Joback Method
dvisc	0.0001653	Pa×s	586.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6380285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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