

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

Other names:	Acetic acid, 2-isopropylphenyl ester
Inchi:	InChI=1S/C11H14O2/c1-8(2)10-6-4-5-7-11(10)13-9(3)12/h4-8H,1-3H3
InchiKey:	ILKITZBHQBDKCB-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]:	178.23
CAS:	1608-68-0

Physical Properties

Property code	Value	Unit	Source
gf	-91.84	kJ/mol	Joback Method
hf	-295.39	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.735		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1277.00		NIST Webbook
tb	558.59	K	Joback Method
tc	773.47	K	Joback Method
tf	309.83	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.51	J/molxK	558.59	Joback Method
cpg	411.28	J/molxK	737.66	Joback Method
cpg	399.87	J/molxK	701.84	Joback Method
cpg	387.70	J/molxK	666.03	Joback Method
cpg	374.76	J/molxK	630.22	Joback Method
cpg	361.03	J/molxK	594.40	Joback Method
cpg	421.95	J/molxK	773.47	Joback Method

dvisc	0.0001834	Paxs	558.59	Joback Method
dvisc	0.0002352	Paxs	517.13	Joback Method
dvisc	0.0003151	Paxs	475.67	Joback Method
dvisc	0.0004464	Paxs	434.21	Joback Method
dvisc	0.0006805	Paxs	392.75	Joback Method
dvisc	0.0011460	Paxs	351.29	Joback Method
dvisc	0.0022187	Paxs	309.83	Joback Method

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=C1608680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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