Phenol, 2,6-dimethoxy-, acetate

Other names:	2-Acetyl-1,3-dimethylpyrogallol
	2,6-Dimethoxyphenylacetate
	Acetic acid, 2,6-dimethoxyphenyl ester
	2,6-Dimethoxyphenol, acetate
Inchi:	InChI=1S/C10H12O4/c1-7(11)14-10-8(12-2)5-4-6-9(10)13-3/h4-6H,1-3H3
InchiKey:	CIIHIFFNYMLOAV-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COc1cccc(OC)c1OC(C)=O
Mol. weight [g/mol]:	196.20
CAS:	944-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-317.45	kJ/mol	Joback Method
hf	-545.38	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.629		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1482.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	585.97	K	Joback Method
tc	796.18	K	Joback Method
tf	370.54	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.19	J/mol×K	585.97	Joback Method
cpg	404.44	J/mol×K	761.14	Joback Method
cpg	394.23	J/mol×K	726.11	Joback Method

cpg	383.37	J/mol×K	691.07	Joback Method
cpg	371.90	J/mol×K	656.04	Joback Method
cpg	359.83	J/mol×K	621.00	Joback Method
cpg	413.99	J/mol×K	796.18	Joback Method
dvisc	0.0001372	Pa×s	585.97	Joback Method
dvisc	0.0001676	Pa×s	550.07	Joback Method
dvisc	0.0002105	Pa×s	514.16	Joback Method
dvisc	0.0002736	Pa×s	478.25	Joback Method
dvisc	0.0003711	Pa×s	442.35	Joback Method
dvisc	0.0005311	Pa×s	406.45	Joback Method
dvisc	0.0008149	Pa×s	370.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C944990&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume