3-Methylcatechol, diacetate

Inchi: InChI=1S/C11H12O4/c1-7-5-4-6-10(14-8(2)12)11(7)15-9(3)13/h4-6H,1-3H3
InchiKey: WSDQZFOBIKMDJE-UHFFFAOYSA-N
Formula: C11H12O4
SMILES: CC(=O)Oc1cccc(C)c1OC(C)=O
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
gf	-332.95	kJ/mol	Joback Method
hf	-546.38	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.846		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1452.50		NIST Webbook
tb	640.30	K	Joback Method
tc	856.49	K	Joback Method
tf	409.51	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.86	J/mol×K	640.30	Joback Method
cpg	441.07	J/mol×K	820.46	Joback Method
cpg	431.51	J/mol×K	784.43	Joback Method
cpg	421.20	J/mol×K	748.40	Joback Method
cpg	410.14	J/mol×K	712.36	Joback Method
cpg	398.36	J/mol×K	676.33	Joback Method
cpg	449.88	J/mol×K	856.49	Joback Method
dvisc	0.0001637	Pa×s	640.30	Joback Method
dvisc	0.0002001	Pa×s	601.84	Joback Method

dvisc	0.0002515	Pa×s	563.37	Joback Method
dvisc	0.0003268	Pa×s	524.90	Joback Method
dvisc	0.0004426	Pa×s	486.44	Joback Method
dvisc	0.0006315	Pa×s	447.97	Joback Method
dvisc	0.0009633	Pa×s	409.51	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=U352789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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