4-tert-Butyl-O-phenylene diacetate

Other names: 4-tert-Butylcatechol, diacetate
4-tert-Butyl-1,2-diacetoxybenzene
2-(Acetyloxy)-4-tert-butylphenyl acetate
Inchi: InChI=1S/C14H18O4/c1-9(15)17-12-7-6-11(14(3,4)5)8-13(12)18-10(2)16/h6-8H,1-5H3
InchiKey: NBDHUKNVZPIOEW-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CC(=O)Oc1ccc(C(C)(C)C)cc1OC(C)=O
Mol. weight [g/mol]: 250.29
CAS: 80869-94-9

Physical Properties

Property code	Value	Unit	Source
gf	-304.85	kJ/mol	Joback Method
hf	-617.05	kJ/mol	Joback Method
hfus	23.44	kJ/mol	Joback Method
hvap	67.37	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.835		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1663.50		NIST Webbook
tb	705.71	K	Joback Method
tc	922.82	K	Joback Method
tf	445.74	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.74	J/mol×K	705.71	Joback Method
cpg	556.41	J/mol×K	741.90	Joback Method
cpg	570.09	J/mol×K	778.08	Joback Method
cpg	582.79	J/mol×K	814.27	Joback Method
cpg	594.55	J/mol×K	850.45	Joback Method

cpg	605.37	J/mol×K	886.64	Joback Method
cpg	615.29	J/mol×K	922.82	Joback Method
dvisc	0.0008100	Pa×s	445.74	Joback Method
dvisc	0.0004893	Pa×s	489.07	Joback Method
dvisc	0.0003208	Pa×s	532.40	Joback Method
dvisc	0.0002241	Pa×s	575.73	Joback Method
dvisc	0.0001647	Pa×s	619.05	Joback Method
dvisc	0.0001259	Pa×s	662.38	Joback Method
dvisc	0.0000995	Pa×s	705.71	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80869949&Units=SI

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