1-Propanone, 2,2-dimethyl-1-(4-phenoxyphenyl)-

Other names: 4'-Phenoxypivalophenone
tert-Butyl 4-phenoxyphenyl ketone
Inchi: InChI=1S/C17H18O2/c1-17(2,3)16(18)13-9-11-15(12-10-13)19-14-7-5-4-6-8-14/h4-12H,1
InchiKey: ITEMAFJPIQQQMO-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: CC(C)(C)C(=O)c1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 254.32
CAS: 55814-54-5

Physical Properties

Property code	Value	Unit	Source
gf	76.37	kJ/mol	Joback Method
hf	-186.17	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	66.51	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.708		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
tb	719.76	K	Joback Method
tc	962.04	K	Joback Method
tf	421.29	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.82	J/mol×K	719.76	Joback Method
cpg	645.14	J/mol×K	921.66	Joback Method
cpg	633.29	J/mol×K	881.28	Joback Method
cpg	620.32	J/mol×K	840.90	Joback Method
cpg	606.15	J/mol×K	800.52	Joback Method
cpg	590.68	J/mol×K	760.14	Joback Method
cpg	655.96	J/mol×K	962.04	Joback Method

dvisc	0.0000906	Pa×s	719.76	Joback Method
dvisc	0.0001177	Pa×s	670.01	Joback Method
dvisc	0.0001595	Pa×s	620.27	Joback Method
dvisc	0.0002278	Pa×s	570.52	Joback Method
dvisc	0.0003482	Pa×s	520.78	Joback Method
dvisc	0.0005824	Pa×s	471.04	Joback Method
dvisc	0.0010996	Pa×s	421.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.20	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55814545&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

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume