

p-tert-Butylpivalophenone

Inchi:	InChI=1S/C15H22O/c1-14(2,3)12-9-7-11(8-10-12)13(16)15(4,5)6/h7-10H,1-6H3
InchiKey:	ZISXBXYWRHTLEN-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC(C)(C)C(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	218.33
CAS:	22583-66-0

Physical Properties

Property code	Value	Unit	Source
gf	54.96	kJ/mol	Joback Method
hf	-257.95	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.213		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
tb	621.67	K	Joback Method
tc	845.21	K	Joback Method
tf	352.52	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.18	J/molxK	621.67	Joback Method
cpg	542.88	J/molxK	658.93	Joback Method
cpg	560.23	J/molxK	696.18	Joback Method
cpg	576.34	J/molxK	733.44	Joback Method
cpg	591.30	J/molxK	770.69	Joback Method
cpg	605.19	J/molxK	807.95	Joback Method
cpg	618.12	J/molxK	845.21	Joback Method
dvisc	0.0026051	Paxs	352.52	Joback Method
dvisc	0.0011955	Paxs	397.38	Joback Method

dvisc	0.0006426	Paxs	442.24	Joback Method
dvisc	0.0003872	Paxs	487.10	Joback Method
dvisc	0.0002541	Paxs	531.95	Joback Method
dvisc	0.0001781	Paxs	576.81	Joback Method
dvisc	0.0001314	Paxs	621.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.50 ± 1.50	K	0.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C22583660&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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