Benzoyl chloride, 4-(1,1-dimethylethyl)-

Other names: 4-tert-Butylbenzoyl chloride
p-tert-Butylbenzoyl chloride
Inchi: InChI=1S/C11H13ClO/c1-11(2,3)9-6-4-8(5-7-9)10(12)13/h4-7H,1-3H3
InchiKey: WNLMYNASWOULQY-UHFFFAOYSA-N
Formula: C11H13ClO
SMILES: CC(C)(C)c1ccc(C(=O)Cl)cc1
Mol. weight [g/mol]: 196.67
CAS: 1710-98-1

Physical Properties

Property code	Value	Unit	Source
gf	6.51	kJ/mol	Joback Method
hf	-182.38	kJ/mol	Joback Method
hfus	16.28	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
ie	9.14	eV	NIST Webbook
log10ws	-3.67		Crippen Method
logp	3.363		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	1112.00		NIST Webbook
tb	570.81	K	Joback Method
tc	801.60	K	Joback Method
tf	334.94	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.13	J/mol×K	570.81	Joback Method
cpg	366.57	J/mol×K	609.27	Joback Method
cpg	379.94	J/mol×K	647.74	Joback Method
cpg	392.30	J/mol×K	686.20	Joback Method
cpg	403.73	J/mol×K	724.67	Joback Method

cpg	414.29	J/mol×K	763.13	Joback Method
cpg	424.04	J/mol×K	801.60	Joback Method
dvisc	0.0025092	Pa×s	334.94	Joback Method
dvisc	0.0013458	Pa×s	374.25	Joback Method
dvisc	0.0008126	Pa×s	413.56	Joback Method
dvisc	0.0005356	Pa×s	452.88	Joback Method
dvisc	0.0003773	Pa×s	492.19	Joback Method
dvisc	0.0002799	Pa×s	531.50	Joback Method
dvisc	0.0002164	Pa×s	570.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	2.70	NIST Webbook

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=C1710981&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
ie: Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume