2,4,6-Triisopropylbenzoyl chloride

Other names: Benzoyl chloride, 2,4,6-tris(1-methylethyl)-
Inchi: InChI=1S/C16H23ClO/c1-9(2)12-7-13(10(3)4)15(16(17)18)14(8-12)11(5)6/h7-11H,1-6H3
InchiKey: OSKNTKJPGKHDHV-UHFFFAOYSA-N
Formula: C16H23ClO
SMILES: CC(C)c1cc(C(C)C)c(C(=O)Cl)c(C(C)C)c1
Mol. weight [g/mol]: 266.81
CAS: 57199-00-5

Physical Properties

Property code	Value	Unit	Source
gf	19.19	kJ/mol	Joback Method
hf	-315.61	kJ/mol	Joback Method
hfus	25.30	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.436		Crippen Method
mcvol	226.350	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
tb	697.08	K	Joback Method
tc	910.67	K	Joback Method
tf	368.91	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.18	J/mol×K	697.08	Joback Method
cpg	619.13	J/mol×K	732.68	Joback Method
cpg	635.06	J/mol×K	768.28	Joback Method
cpg	650.00	J/mol×K	803.87	Joback Method
cpg	663.98	J/mol×K	839.47	Joback Method
cpg	677.03	J/mol×K	875.07	Joback Method
cpg	689.20	J/mol×K	910.67	Joback Method
dvisc	0.0019303	Pa×s	368.91	Joback Method

dvisc	0.0008851	Pa×s	423.61	Joback Method
dvisc	0.0004851	Pa×s	478.30	Joback Method
dvisc	0.0003008	Pa×s	533.00	Joback Method
dvisc	0.0002039	Pa×s	587.69	Joback Method
dvisc	0.0001476	Pa×s	642.38	Joback Method
dvisc	0.0001125	Pa×s	697.08	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=C57199005&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume