

2,4,6-Trimethylbenzoyl chloride

Other names:	Benzoyl chloride, 2,4,6-trimethyl-
Inchi:	InChI=1S/C10H11ClO/c1-6-4-7(2)9(10(11)12)8(3)5-6/h4-5H,1-3H3
InchiKey:	UKRQMDIFLKHCRO-UHFFFAOYSA-N
Formula:	C10H11ClO
SMILES:	Cc1cc(C)c(C(=O)Cl)c(C)c1
Mol. weight [g/mol]:	182.65
CAS:	938-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-24.01	kJ/mol	Joback Method
hf	-175.93	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	2.991		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	561.12	K	Joback Method
tc	784.10	K	Joback Method
tf	346.29	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.46	J/mol×K	561.12	Joback Method
cpg	313.59	J/mol×K	598.28	Joback Method
cpg	325.03	J/mol×K	635.45	Joback Method
cpg	335.81	J/mol×K	672.61	Joback Method
cpg	345.94	J/mol×K	709.78	Joback Method
cpg	355.45	J/mol×K	746.94	Joback Method
cpg	364.34	J/mol×K	784.10	Joback Method
dvisc	0.0013634	Pa×s	346.29	Joback Method

dvisc	0.0008965	Pa×s	382.10	Joback Method
dvisc	0.0006334	Pa×s	417.90	Joback Method
dvisc	0.0004728	Pa×s	453.71	Joback Method
dvisc	0.0003683	Pa×s	489.51	Joback Method
dvisc	0.0002968	Pa×s	525.32	Joback Method
dvisc	0.0002459	Pa×s	561.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C938181&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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