Benzoyl chloride, 4-methyl-

Other names:	p-Toluoyl chloride
	p-Methylbenzoyl chloride
	p-Toluic acid chloride
	p-Toluyl chloride
	4-Methylbenzoyl chloride
	4-Toluoyl chloride
	4-Methylbenzoic acid chloride
Inchi:	InChI=1S/C8H7ClO/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3
InchiKey:	NQUVCRCCRXRJCK-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	Cc1ccc(C(=O)Cl)cc1
Mol. weight [g/mol]:	154.59
CAS:	874-60-2

Physical Properties

Property code	Value	Unit	Source
gf	-21.59	kJ/mol	Joback Method
hf	-139.70 ± 7.40	kJ/mol	NIST Webbook
hfl	-201.30 ± 6.10	kJ/mol	NIST Webbook
hfus	15.92	kJ/mol	Joback Method
hvap	61.50 ± 4.20	kJ/mol	NIST Webbook
ie	9.37 ± 0.01	eV	NIST Webbook
log10ws	-2.84		Crippen Method
logp	2.374		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	499.20	K	NIST Webbook
tc	734.29	K	Joback Method
tf	298.71	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	216.19	J/mol×K	505.40	Joback Method
cpg	226.80	J/mol×K	543.55	Joback Method
cpg	236.72	J/mol×K	581.70	Joback Method
cpg	245.97	J/mol×K	619.84	Joback Method
cpg	254.59	J/mol×K	657.99	Joback Method
cpg	262.58	J/mol×K	696.14	Joback Method
cpg	270.00	J/mol×K	734.29	Joback Method
dvisc	0.0021784	Pa×s	298.71	Joback Method
dvisc	0.0013126	Pa×s	333.16	Joback Method
dvisc	0.0008697	Pa×s	367.61	Joback Method
dvisc	0.0006184	Pa×s	402.06	Joback Method
dvisc	0.0004640	Pa×s	436.50	Joback Method
dvisc	0.0003631	Pa×s	470.95	Joback Method
dvisc	0.0002938	Pa×s	505.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.00 ± 1.00	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=C874602&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
hfl: Liquid phase 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
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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