Benzoyl chloride, 2-methyl-

Other names:	o-Toluoyl chloride
	o-Methylbenzoyl chloride
	o-Toluic acid chloride
	2-Methylbenzoyl chloride
	2-Toluoyl chloride
	o-Toluyl chloride
Inchi:	InChI=1S/C8H7ClO/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3
InchiKey:	GPZXFICWCMCQPF-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	Cc1ccccc1C(=O)Cl
Mol. weight [g/mol]:	154.59
CAS:	933-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-21.59	kJ/mol	Joback Method
hf	-111.71	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.374		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	505.40	K	Joback Method
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	362.20	K	1.60	NIST Webbook
tbrp	366.50 ± 1.50	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C933880&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

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