Benzoyl chloride, 2-methoxy-

Other names:	o-Anisoyl chloride
	o-Methoxybenzoyl chloride
	2-Methoxybenzoyl chloride
Inchi:	InChI=1S/C8H7ClO2/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3
InchiKey:	RZNHSEZOLFEFGB-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	COc1ccccc1C(=O)Cl
Mol. weight [g/mol]:	170.59
CAS:	21615-34-9

Physical Properties

Property code	Value	Unit	Source
gf	-126.59	kJ/mol	Joback Method
hf	-243.93	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.074		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	527.20	K	NIST Webbook
tc	753.98	K	Joback Method
tf	320.94	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.52	J/mol×K	527.82	Joback Method
cpg	247.94	J/mol×K	565.51	Joback Method
cpg	257.76	J/mol×K	603.21	Joback Method
cpg	266.97	J/mol×K	640.90	Joback Method
cpg	275.58	J/mol×K	678.59	Joback Method
cpg	283.61	J/mol×K	716.28	Joback Method

cpg	291.07	J/mol×K	753.98	Joback Method
dvisc	0.0017026	Pa×s	320.94	Joback Method
dvisc	0.0010543	Pa×s	355.42	Joback Method
dvisc	0.0007106	Pa×s	389.90	Joback Method
dvisc	0.0005107	Pa×s	424.38	Joback Method
dvisc	0.0003857	Pa×s	458.86	Joback Method
dvisc	0.0003030	Pa×s	493.34	Joback Method
dvisc	0.0002456	Pa×s	527.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.70	K	1.00	NIST Webbook
tbrp	401.20	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21615349&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