«alpha»-Chlorophenylacetyl chloride

Other names:	a-Chlorophenylacetyl chloride
	Benzeneacetyl chloride, «alpha»-chloro-
	DL-2-Chloro-2-phenylacetyl chloride
	chloro(phenyl)acetyl chloride
Inchi:	InChI=1S/C8H6Cl2O/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H
InchiKey:	FGEAOSXMQZWHIQ-UHFFFAOYSA-N
Formula:	C8H6Cl2O
SMILES:	O=C(Cl)C(Cl)c1ccccc1
Mol. weight [g/mol]:	189.04
CAS:	2912-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-26.33	kJ/mol	Joback Method
hf	-121.26	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	50.81	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.732		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	537.41	K	Joback Method
tc	775.44	K	Joback Method
tf	301.11	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.85	J/mol×K	537.41	Joback Method
cpg	250.36	J/mol×K	577.08	Joback Method
cpg	260.03	J/mol×K	616.75	Joback Method
cpg	268.93	J/mol×K	656.42	Joback Method
cpg	277.08	J/mol×K	696.09	Joback Method

cpg	284.53	J/mol×K	735.76	Joback Method
cpg	291.33	J/mol×K	775.44	Joback Method
dvisc	0.0036093	Pa×s	301.11	Joback Method
dvisc	0.0018614	Pa×s	340.49	Joback Method
dvisc	0.0011013	Pa×s	379.88	Joback Method
dvisc	0.0007191	Pa×s	419.26	Joback Method
dvisc	0.0005052	Pa×s	458.64	Joback Method
dvisc	0.0003753	Pa×s	498.03	Joback Method
dvisc	0.0002912	Pa×s	537.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	3.10	NIST Webbook
tbrp	395.50 ± 2.50	K	2.70	NIST Webbook

Sources

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=C2912621&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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