p-Chlorophenylacetyl chloride

Other names:	4-Chlorophenacyl chloride
	4-Chlorophenylacetyl chloride
	Benzeneacetyl chloride, 4-chloro-
Inchi:	InChI=1S/C8H6Cl2O/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2
InchiKey:	UMQUIRYNOVNYPA-UHFFFAOYSA-N
Formula:	C8H6Cl2O
SMILES:	O=C(Cl)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	189.04
CAS:	25026-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-33.52	kJ/mol	Joback Method
hf	-127.45	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.648		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	542.83	K	Joback Method
tc	776.56	K	Joback Method
tf	328.63	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.61	J/mol×K	542.83	Joback Method
cpg	281.02	J/mol×K	737.60	Joback Method
cpg	273.83	J/mol×K	698.65	Joback Method
cpg	266.02	J/mol×K	659.69	Joback Method
cpg	257.58	J/mol×K	620.74	Joback Method
cpg	248.45	J/mol×K	581.78	Joback Method

cpg	287.64	J/mol×K	776.56	Joback Method
dvisc	0.0003006	Pa×s	542.83	Joback Method
dvisc	0.0003716	Pa×s	507.13	Joback Method
dvisc	0.0004744	Pa×s	471.43	Joback Method
dvisc	0.0006303	Pa×s	435.73	Joback Method
dvisc	0.0008809	Pa×s	400.03	Joback Method
dvisc	0.0013147	Pa×s	364.33	Joback Method
dvisc	0.0021405	Pa×s	328.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.50 ± 1.50	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=C25026340&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