4-(Chloromethyl)benzoyl chloride

Other names: Benzoyl chloride, 4-(chloromethyl)-
Inchi: InChI=1S/C8H6Cl2O/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4H,5H2
InchiKey: RCOVTJVRTZGSBP-UHFFFAOYSA-N
Formula: C8H6Cl2O
SMILES: O=C(Cl)c1ccc(CCl)cc1
Mol. weight [g/mol]: 189.04
CAS: 876-08-4

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	-3.39		Crippen Method
logp	2.804		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	287.64	J/mol×K	776.56	Joback Method
cpg	238.61	J/mol×K	542.83	Joback Method
cpg	248.45	J/mol×K	581.78	Joback Method
cpg	257.58	J/mol×K	620.74	Joback Method
cpg	266.02	J/mol×K	659.69	Joback Method
cpg	273.83	J/mol×K	698.65	Joback Method
cpg	281.02	J/mol×K	737.60	Joback Method
dvisc	0.0003006	Pa×s	542.83	Joback Method

dvisc	0.0021405	Pa×s	328.63	Joback Method
dvisc	0.0013147	Pa×s	364.33	Joback Method
dvisc	0.0008809	Pa×s	400.03	Joback Method
dvisc	0.0006303	Pa×s	435.73	Joback Method
dvisc	0.0004744	Pa×s	471.43	Joback Method
dvisc	0.0003716	Pa×s	507.13	Joback Method
hvapt	68.30	kJ/mol	453.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.83918e+01
Coeff. B	-7.49030e+03
Temperature range (K), min.	413.73
Temperature range (K), max.	572.64

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=C876084&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume