Benzeneacetyl chloride

Other names:	Acetyl chloride, phenyl-
	Phenacetyl chloride
	Phenylacetic acid chloride
	Phenylacetyl chloride
	UN 2577
	«alpha»-Phenylacetyl chloride
	Â«alphaÂ»-Phenylacetyl chloride
Inchi:	InChI=1S/C8H7ClO/c9-8(10)6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	VMZCDNSFRSVYKQ-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	O=C(Cl)Cc1ccccc1
Mol. weight [g/mol]:	154.59
CAS:	103-80-0

Physical Properties

Property code	Value	Unit	Source
gf	-11.96	kJ/mol	Joback Method
hf	-100.24	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.994		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	482.00 ± 8.00	K	NIST Webbook
tc	728.04	K	Joback Method
tf	286.19	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.90	J/mol×K	728.04	Joback Method
cpg	264.36	J/mol×K	690.11	Joback Method

cpg	256.20	J/mol×K	652.17	Joback Method
cpg	247.37	J/mol×K	614.23	Joback Method
cpg	237.84	J/mol×K	576.29	Joback Method
cpg	227.58	J/mol×K	538.36	Joback Method
cpg	216.55	J/mol×K	500.42	Joback Method
dvisc	0.0029389	Pa×s	286.19	Joback Method
dvisc	0.0003049	Pa×s	500.42	Joback Method
dvisc	0.0003848	Pa×s	464.71	Joback Method
dvisc	0.0005047	Pa×s	429.01	Joback Method
dvisc	0.0006953	Pa×s	393.30	Joback Method
dvisc	0.0010214	Pa×s	357.60	Joback Method
dvisc	0.0016339	Pa×s	321.89	Joback Method
hvapt	56.50	kJ/mol	402.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.70	K	1.60	NIST Webbook
tbrp	443.20	K	33.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52019e+01
Coeff. B	-4.54533e+03
Coeff. C	-5.79100e+01
Temperature range (K), min.	362.67
Temperature range (K), max.	517.48

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103800&Units=SI

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

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume