Cinnamoyl chloride

Other names:	2-Propenoyl chloride, 3-phenyl-
	«beta»-Phenylacryloyl chloride
	Cinnamic acid chloride
	Cinnamic chloride
	3-Phenyl-2-propenoyl chloride
	3-Phenylacryloyl chloride
	NSC 4683
Inchi:	InChI=1S/C9H7ClO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H/b7-6+
InchiKey:	WOGITNXCNOTRLK-VOTSOKGWSA-N
Formula:	C9H7ClO
SMILES:	O=C(Cl)C=Cc1ccccc1
Mol. weight [g/mol]:	166.60
CAS:	102-92-1

Physical Properties

Property code	Value	Unit	Source
gf	76.68	kJ/mol	Joback Method
hf	-3.66	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.465		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	240.50		NIST Webbook
tb	530.20	K	NIST Webbook
tc	761.93	K	Joback Method
tf	292.38	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.31	J/mol×K	527.46	Joback Method

cpg	289.13	J/mol×K	722.85	Joback Method
cpg	280.93	J/mol×K	683.77	Joback Method
cpg	272.01	J/mol×K	644.70	Joback Method
cpg	262.30	J/mol×K	605.62	Joback Method
cpg	251.76	J/mol×K	566.54	Joback Method
cpg	296.67	J/mol×K	761.93	Joback Method
dvisc	0.0002418	Pa×s	527.46	Joback Method
dvisc	0.0003078	Pa×s	488.28	Joback Method
dvisc	0.0004085	Pa×s	449.10	Joback Method
dvisc	0.0005724	Pa×s	409.92	Joback Method
dvisc	0.0008614	Pa×s	370.74	Joback Method
dvisc	0.0014276	Pa×s	331.56	Joback Method
dvisc	0.0027090	Pa×s	292.38	Joback Method

Sources

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=C102921&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume