3-Phenylpropionyl chloride

Other names:	3-Phenylpropanoyl chloride
	3-Phenylpropionic acid chloride
	3-Phenylpropionyl chloride
	Dihydrocinnamoyl chloride
	Hydrocinnamoyl chloride
	Hydrocinnamyl chloride
	NSC 2854
	Propionyl chloride, 3-phenyl-
	«beta»-Phenylpropanoyl chloride
	«beta»-Phenylpropionyl chloride
Inchi:	InChI=1S/C9H9ClO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	MFEILWXBDBCWKF-UHFFFAOYSA-N
Formula:	C9H9ClO
SMILES:	O=C(Cl)CCc1ccccc1
Mol. weight [g/mol]:	168.62

Physical Properties

Property code	Value	Unit	Source
af	0.4382		Cheméo Relay (1.0)
gf	-3.54	kJ/mol	Joback Method
hf	-119.85	kJ/mol	Cheméo Relay (1.0)
hfus	18.90	kJ/mol	Joback Method
hvap	54.66	kJ/mol	Cheméo Relay (1.0)
ie	9.28	eV	Cheméo Relay (1.0)
log10ws	-2.48		Cheméo Relay (1.0)
logp	2.385		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1280.50		NIST Webbook
tb	502.33	K	Cheméo Relay (1.0)
tc	718.43	K	Cheméo Relay (1.0)
tf	250.49	K	Cheméo Relay (1.0)
vc	0.449	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.91	J/mol×K	523.30	Joback Method
cpg	271.02	J/mol×K	560.57	Joback Method
cpg	282.32	J/mol×K	597.85	Joback Method
cpg	292.84	J/mol×K	635.12	Joback Method
cpg	302.62	J/mol×K	672.39	Joback Method
cpg	311.69	J/mol×K	709.67	Joback Method
cpg	320.10	J/mol×K	746.94	Joback Method
dvisc	0.0029503	Pa×s	297.46	Joback Method
dvisc	0.0016071	Pa×s	335.10	Joback Method
dvisc	0.0009896	Pa×s	372.74	Joback Method
dvisc	0.0006661	Pa×s	410.38	Joback Method
dvisc	0.0004792	Pa×s	448.02	Joback Method
dvisc	0.0003628	Pa×s	485.66	Joback Method
dvisc	0.0002859	Pa×s	523.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	1.50	NIST Webbook
tbrp	389.50 ± 0.50	K	2.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C645454&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume