1-propanone, 3-chloro-2-(chloromethyl)-1-phenyl-

Other names: 3-chloro-2-(chloromethyl)-1-phenylpropan-1-one
1-Phenyl-3-chloro-2-(chloromethyl)-1-propanone

Inchi: InChI=1S/C10H10Cl2O/c11-6-9(7-12)10(13)8-4-2-1-3-5-8/h1-5,9H,6-7H2

InchiKey: SJJAYVWBFICAEB-UHFFFAOYSA-N

Formula: C10H10Cl2O

SMILES: O=C(c1ccccc1)C(CCl)CCl

Mol. weight [g/mol]: 217.09

Physical Properties

Property code	Value	Unit	Source
gf	-9.49	kJ/mol	Joback Method
hf	-162.54	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.963		Crippen Method
mcvol	154.050	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	583.17	K	Joback Method
tc	811.98	K	Joback Method
tf	323.65	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.60	J/mol×K	583.17	Joback Method
cpg	341.03	J/mol×K	621.30	Joback Method
cpg	352.56	J/mol×K	659.44	Joback Method
cpg	363.22	J/mol×K	697.57	Joback Method
cpg	373.07	J/mol×K	735.71	Joback Method
cpg	382.15	J/mol×K	773.84	Joback Method

cpg	390.52	J/mol×K	811.98	Joback Method
dvisc	0.0033436	Pa×s	323.65	Joback Method
dvisc	0.0016662	Pa×s	366.90	Joback Method
dvisc	0.0009617	Pa×s	410.16	Joback Method
dvisc	0.0006165	Pa×s	453.41	Joback Method
dvisc	0.0004270	Pa×s	496.66	Joback Method
dvisc	0.0003137	Pa×s	539.92	Joback Method
dvisc	0.0002412	Pa×s	583.17	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=U400729&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

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