

1-(2-Chlorophenyl)propan-2-one

Inchi:	InChI=1S/C9H9ClO/c1-7(11)6-8-4-2-3-5-9(8)10/h2-5H,6H2,1H3
InchiKey:	LWGNNDIMNCPMZOF-UHFFFAOYSA-N
Formula:	C9H9ClO
SMILES:	CC(=O)Cc1ccccc1Cl
Mol. weight [g/mol]:	168.62
CAS:	6305-95-9

Physical Properties

Property code	Value	Unit	Source
gf	-13.17	kJ/mol	Joback Method
hf	-132.35	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.471		Crippen Method
mvol	127.720	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	528.28	K	Joback Method
tc	753.10	K	Joback Method
tf	309.98	K	Joback Method
vc	0.486	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.49	J/molxK	528.28	Joback Method
cpg	270.24	J/molxK	565.75	Joback Method
cpg	281.24	J/molxK	603.22	Joback Method
cpg	291.51	J/molxK	640.69	Joback Method
cpg	301.10	J/molxK	678.16	Joback Method
cpg	310.02	J/molxK	715.63	Joback Method
cpg	318.31	J/molxK	753.10	Joback Method
dvisc	0.0022080	Paxs	309.98	Joback Method
dvisc	0.0013025	Paxs	346.36	Joback Method

dvisc	0.0008494	Paxs	382.75	Joback Method
dvisc	0.0005966	Paxs	419.13	Joback Method
dvisc	0.0004434	Paxs	455.51	Joback Method
dvisc	0.0003443	Paxs	491.90	Joback Method
dvisc	0.0002769	Paxs	528.28	Joback Method

Sources

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=C6305959&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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