4-Chlorophenyl cyclopropyl ketone

Other names: Methanone, (4-chlorophenyl)cyclopropyl-
Inchi: InChI=1S/C10H9ClO/c11-9-5-3-8(4-6-9)10(12)7-1-2-7/h3-7H,1-2H2
InchiKey: OPSFCTBBDIDFJM-UHFFFAOYSA-N
Formula: C10H9ClO
SMILES: O=C(c1ccc(Cl)cc1)C1CC1
Mol. weight [g/mol]: 180.63
CAS: 6640-25-1

Physical Properties

Property code	Value	Unit	Source
gf	56.00	kJ/mol	Joback Method
hf	-80.19	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	51.84	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.933		Crippen Method
mcvol	130.950	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	557.90	K	Joback Method
tc	795.94	K	Joback Method
tf	339.19	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.71	J/mol×K	557.90	Joback Method
cpg	301.08	J/mol×K	597.57	Joback Method
cpg	313.40	J/mol×K	637.25	Joback Method
cpg	324.75	J/mol×K	676.92	Joback Method
cpg	335.20	J/mol×K	716.59	Joback Method
cpg	344.83	J/mol×K	756.26	Joback Method
cpg	353.72	J/mol×K	795.94	Joback Method
dvisc	0.0021340	Pa×s	339.19	Joback Method

dvisc	0.0015419	Pa×s	375.64	Joback Method
dvisc	0.0011801	Pa×s	412.09	Joback Method
dvisc	0.0009432	Pa×s	448.54	Joback Method
dvisc	0.0007798	Pa×s	485.00	Joback Method
dvisc	0.0006620	Pa×s	521.45	Joback Method
dvisc	0.0005742	Pa×s	557.90	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=C6640251&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
mcvol:	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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