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

Physical Properties

Property code	Value	Unit	Source
hf	-75.42	kJ/mol	Cheméo Relay (1.0)
hfus	19.24	kJ/mol	Joback Method
hvap	73.03	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-3.65		Cheméo Relay (1.0)
logp	2.933		Crippen Method
mcvol	130.950	ml/mol	McGowan Method
tb	545.24	K	Cheméo Relay (1.0)
tf	346.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.71	J/mol×K	557.90	Joback Method
cpg	353.72	J/mol×K	795.94	Joback Method
cpg	344.83	J/mol×K	756.26	Joback Method
cpg	335.20	J/mol×K	716.59	Joback Method
cpg	324.75	J/mol×K	676.92	Joback Method
cpg	313.40	J/mol×K	637.25	Joback Method
cpg	301.08	J/mol×K	597.57	Joback Method
dvisc	0.0009432	Pa×s	448.54	Joback Method
dvisc	0.0005742	Pa×s	557.90	Joback Method
dvisc	0.0006620	Pa×s	521.45	Joback Method
dvisc	0.0007798	Pa×s	485.00	Joback Method
dvisc	0.0021340	Pa×s	339.19	Joback Method

dvisc	0.0011801	Pa×s	412.09	Joback Method
dvisc	0.0015419	Pa×s	375.64	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640251&Units=SI

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):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point