4-CHLOROBUTYROPHENONE

Other names: 4-Chlorobutyrophenone
«omega»-Chlorobutyrophenone
1-Butanone, 4-chloro-1-phenyl-
Inchi: InChI=1S/C10H11ClO/c11-8-4-7-10(12)9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2
InchiKey: GHEFQKHLHFXSBR-UHFFFAOYSA-N
Formula: C10H11ClO
SMILES: O=C(CCCCl)c1ccccc1
Mol. weight [g/mol]: 182.65

Physical Properties

Property code	Value	Unit	Source
af	0.5069		Cheméo Relay (1.0)
gf	4.88	kJ/mol	Joback Method
hf	-157.96	kJ/mol	Cheméo Relay (1.0)
hfus	21.49	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.888		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	540.30	K	Cheméo Relay (1.0)
tc	768.42	K	Cheméo Relay (1.0)
tf	292.51	K	Cheméo Relay (1.0)
vc	0.500	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.13	J/mol×K	546.18	Joback Method
cpg	316.19	J/mol×K	582.80	Joback Method
cpg	328.40	J/mol×K	619.42	Joback Method
cpg	339.78	J/mol×K	656.04	Joback Method
cpg	350.39	J/mol×K	692.66	Joback Method

cpg	360.25	J/mol×K	729.28	Joback Method
cpg	369.41	J/mol×K	765.90	Joback Method
dvisc	0.0029165	Pa×s	308.73	Joback Method
dvisc	0.0015584	Pa×s	348.31	Joback Method
dvisc	0.0009463	Pa×s	387.88	Joback Method
dvisc	0.0006302	Pa×s	427.45	Joback Method
dvisc	0.0004496	Pa×s	467.03	Joback Method
dvisc	0.0003382	Pa×s	506.60	Joback Method
dvisc	0.0002651	Pa×s	546.18	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C939526&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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume