

«gamma»-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
CAS:	939-52-6

Physical Properties

Property code	Value	Unit	Source
gf	4.88	kJ/mol	Joback Method
hf	-141.52	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	51.26	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.888		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	546.18	K	Joback Method
tc	765.90	K	Joback Method
tf	308.73	K	Joback Method
vc	0.542	m3/kmol	Joback Method

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

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=C939526&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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