

Methanone, (3-chlorophenyl)phenyl-

Other names:	Benzophenone, 3-chloro- m-Chlorobenzophenone 3-Chlorobenzophenone
Inchi:	InChI=1S/C13H9ClO/c14-12-8-4-7-11(9-12)13(15)10-5-2-1-3-6-10/h1-9H
InchiKey:	CPLWKNRPZVNELG-UHFFFAOYSA-N
Formula:	C13H9ClO
SMILES:	O=C(c1ccccc1)c1cccc(Cl)c1
Mol. weight [g/mol]:	216.66
CAS:	1016-78-0

Physical Properties

Property code	Value	Unit	Source
ea	0.87 ± 0.09	eV	NIST Webbook
gf	132.92	kJ/mol	Joback Method
hf	21.62	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hsub	110.40 ± 0.40	kJ/mol	NIST Webbook
hvap	60.88	kJ/mol	Joback Method
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
log10ws	-4.11		Crippen Method
logp	3.571		Crippen Method
mvol	160.320	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	646.48	K	Joback Method
tc	902.74	K	Joback Method
tf	381.48	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.91	J/mol×K	646.48	Joback Method
cpg	379.51	J/mol×K	689.19	Joback Method

cpg	391.90	J/mol×K	731.90	Joback Method
cpg	403.17	J/mol×K	774.61	Joback Method
cpg	413.40	J/mol×K	817.32	Joback Method
cpg	422.66	J/mol×K	860.03	Joback Method
cpg	431.03	J/mol×K	902.74	Joback Method
dvisc	0.0016421	Paxs	381.48	Joback Method
dvisc	0.0009615	Paxs	425.65	Joback Method
dvisc	0.0006226	Paxs	469.81	Joback Method
dvisc	0.0004344	Paxs	513.98	Joback Method
dvisc	0.0003209	Paxs	558.15	Joback Method
dvisc	0.0002478	Paxs	602.31	Joback Method
dvisc	0.0001982	Paxs	646.48	Joback Method
hsubt	108.80 ± 0.40	kJ/mol	330.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1016780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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