2-Chloro-1-(4-chlorophenyl)ethanone

Other names: 2,4'-dichloroacetophenone
Inchi: InChI=1S/C8H6Cl2O/c9-5-8(11)6-1-3-7(10)4-2-6/h1-4H,5H2
InchiKey: FWDFNLVLIXAOMX-UHFFFAOYSA-N
Formula: C8H6Cl2O
SMILES: O=C(CCl)c1ccc(Cl)cc1
Mol. weight [g/mol]: 189.04
CAS: 937-20-2

Physical Properties

Property code	Value	Unit	Source
gf	-33.52	kJ/mol	Joback Method
hf	-127.45	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.761		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	542.83	K	Joback Method
tc	776.56	K	Joback Method
tf	328.63	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.64	J/mol×K	776.56	Joback Method
cpg	248.45	J/mol×K	581.78	Joback Method
cpg	257.58	J/mol×K	620.74	Joback Method
cpg	266.02	J/mol×K	659.69	Joback Method
cpg	273.83	J/mol×K	698.65	Joback Method
cpg	281.02	J/mol×K	737.60	Joback Method
cpg	238.61	J/mol×K	542.83	Joback Method
dvisc	0.0003716	Pa×s	507.13	Joback Method

dvisc	0.0004744	Pa×s	471.43	Joback Method
dvisc	0.0006303	Pa×s	435.73	Joback Method
dvisc	0.0008809	Pa×s	400.03	Joback Method
dvisc	0.0013147	Pa×s	364.33	Joback Method
dvisc	0.0003006	Pa×s	542.83	Joback Method
dvisc	0.0021405	Pa×s	328.63	Joback Method
psub	2.21e-04	kPa	309.18	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.78e-04	kPa	307.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.34e-04	kPa	305.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	9.90e-05	kPa	303.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	8.50e-05	kPa	301.20	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.12e-03	kPa	323.09	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	9.03e-04	kPa	321.15	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	6.99e-04	kPa	319.18	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	5.61e-04	kPa	317.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone

psub	4.47e-04	kPa	315.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	3.44e-04	kPa	313.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	2.78e-04	kPa	311.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	2.18e-04	kPa	309.18	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.65e-04	kPa	307.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.33e-04	kPa	305.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.05e-04	kPa	303.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	7.60e-05	kPa	301.20	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.11e-03	kPa	323.09	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	8.75e-04	kPa	321.15	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone

psub	6.86e-04	kPa	319.18	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	5.53e-04	kPa	317.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	4.37e-04	kPa	315.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	3.41e-04	kPa	313.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	2.71e-04	kPa	311.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	2.14e-04	kPa	309.18	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.65e-04	kPa	307.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.31e-04	kPa	305.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.03e-04	kPa	303.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	7.90e-05	kPa	301.20	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone

psub	3.59e-04	kPa	313.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	4.48e-04	kPa	315.19	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	5.62e-04	kPa	317.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	7.57e-04	kPa	319.18	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	9.11e-04	kPa	321.15	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	1.13e-03	kPa	323.09	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone
psub	2.70e-04	kPa	311.10	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C937202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone:	https://www.doi.org/10.1016/j.jct.2013.07.026
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
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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume