Benzoic acid, 4-chloro-, methyl ester

Other names:	4-Chlorobenzoic acid methyl ester
	Benzoic acid, p-chloro-, methyl ester
	Methyl 4-chlorobenzoate
	Methyl ester of p-chlorobenzoic acid
	Methyl p-chlorobenzoate
Inchi:	InChI=1S/C8H7ClO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,1H3
InchiKey:	LXNFVVDCCWUUKC-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	COC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	170.59
CAS:	1126-46-1

Physical Properties

Property code	Value	Unit	Source
affp	842.10	kJ/mol	NIST Webbook
basg	811.10	kJ/mol	NIST Webbook
gf	-126.59	kJ/mol	Joback Method
hf	-305.00 ± 11.00	kJ/mol	NIST Webbook
hfl	-385.30 ± 2.20	kJ/mol	NIST Webbook
hfus	17.11	kJ/mol	Joback Method
hvap	81.00 ± 10.00	kJ/mol	NIST Webbook
ie	9.57	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	2.127		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1849.00		NIST Webbook

ripol	1859.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1834.00		NIST Webbook
tb	527.82	K	Joback Method
tc	753.98	K	Joback Method
tf	315.13	K	The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.52	J/mol×K	527.82	Joback Method
cpg	283.61	J/mol×K	716.28	Joback Method
cpg	275.58	J/mol×K	678.59	Joback Method
cpg	266.97	J/mol×K	640.90	Joback Method
cpg	257.76	J/mol×K	603.21	Joback Method
cpg	247.94	J/mol×K	565.51	Joback Method
cpg	291.07	J/mol×K	753.98	Joback Method
dvisc	0.0002456	Pa×s	527.82	Joback Method
dvisc	0.0003030	Pa×s	493.34	Joback Method
dvisc	0.0003857	Pa×s	458.86	Joback Method
dvisc	0.0005107	Pa×s	424.38	Joback Method
dvisc	0.0007106	Pa×s	389.90	Joback Method
dvisc	0.0010543	Pa×s	355.42	Joback Method
dvisc	0.0017026	Pa×s	320.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids:	https://www.doi.org/10.1016/j.jct.2012.07.027
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=C1126461&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume