2-Chloroanisole

Other names:	1-chloro-2-methoxybenzene
	2-Chlorophenol methyl ether
	NSC 155175
	anisole, o-chloro-
	benzene, 1-chloro-2-methoxy-
	o-Chloromethoxybenzene
	o-Chlorophenyl methyl ether
	o-chloroanisole
	ortho-Chloroanisole
Inchi:	InChI=1S/C7H7ClO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	QGRPVMLBTFGQDQ-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	COc1ccccc1Cl
Mol. weight [g/mol]:	142.59
CAS:	766-51-8

Physical Properties

Property code	Value	Unit	Source
af	0.3621		Cheméo Relay (1.0)
gf	-6.09	kJ/mol	Joback Method
hf	-109.94	kJ/mol	Cheméo Relay (1.0)
hfus	12.92	kJ/mol	Joback Method
hvap	55.00 ± 0.80	kJ/mol	NIST Webbook
ie	8.30 ± 0.15	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	-2.46		Aqueous Solubility Prediction Method
log10ws	-2.46		Estimated Solubility Method
logp	2.349		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1092.60		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1093.00		NIST Webbook

rinpol	1135.60		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1097.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	468.70	K	NIST Webbook
tc	688.87	K	Cheméo Relay (1.0)
tf	246.35	K	Aqueous Solubility Prediction Method
tf	246.59 ± 0.05	K	NIST Webbook
vc	0.373	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.68	J/mol×K	451.07	Joback Method
cpg	194.76	J/mol×K	487.66	Joback Method
cpg	204.32	J/mol×K	524.25	Joback Method
cpg	213.38	J/mol×K	560.84	Joback Method
cpg	221.95	J/mol×K	597.42	Joback Method
cpg	230.02	J/mol×K	634.01	Joback Method
cpg	237.62	J/mol×K	670.60	Joback Method
dvisc	0.0017445	Pa×s	259.74	Joback Method
dvisc	0.0010328	Pa×s	291.63	Joback Method
dvisc	0.0006780	Pa×s	323.52	Joback Method
dvisc	0.0004800	Pa×s	355.41	Joback Method
dvisc	0.0003597	Pa×s	387.29	Joback Method
dvisc	0.0002817	Pa×s	419.18	Joback Method
dvisc	0.0002283	Pa×s	451.07	Joback Method
hvapt	55.00	kJ/mol	298.15	Standard molar enthalpies of formation of the three isomers of chloroanisole
hvapt	48.30	kJ/mol	424.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65956e+01
Coeff. B	-5.17639e+03
Coeff. C	-3.34430e+01
Temperature range (K), min.	350.86
Temperature range (K), max.	492.18

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Cheméo Relay (1.0):

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C766518&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Standard molar enthalpies of formation of the three isomers of chloroanisole: https://www.doi.org/10.1016/j.jct.2007.10.001

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

hvapt: Enthalpy of vaporization at a given temperature

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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