Benzene, 1-chloro-3-methoxy-

Other names:	1-Chloro-3-methoxybenzene
	3-Chloroanisole
	Anisole, m-chloro-
	m-Chloroanisole
	m-Chlorophenyl methyl ether
	meta-Chloroanisole
Inchi:	InChI=1S/C7H7ClO/c1-9-7-4-2-3-6(8)5-7/h2-5H,1H3
InchiKey:	YUKILTJWFRTXGB-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	COc1cccc(Cl)c1
Mol. weight [g/mol]:	142.58
CAS:	2845-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-6.09	kJ/mol	Joback Method
hf	-110.71	kJ/mol	Joback Method
hfus	12.92	kJ/mol	Joback Method
hvap	53.60 ± 0.80	kJ/mol	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-2.78		Estimated Solubility Method
log10ws	-2.78		Aqueous Solubility Prediction Method
logp	2.349		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1110.80		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1092.00		NIST Webbook

ripol	1628.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	466.70	K	NIST Webbook
tc	670.60	K	Joback Method
tf	259.74	K	Joback Method
vc	0.387	m3/kmol	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.20	K	1.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2845898&Units=SI

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/22-780-1/Benzene-1-chloro-3-methoxy.pdf
Generated by Cheméo on 2024-04-16 19:14:59.431878538 +0000 UTC m=+15584148.352455853.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.