3,4-Dichloroanisole

Other names:	3,4-Dichloroanizole
	3,4-Dichlorophenol, methyl ether
	Benzene, 1,2-dichloro-4-methoxy
	1,2-Dichloro-4-methoxybenzene
Inchi:	InChI=1S/C7H6Cl2O/c1-10-5-2-3-6(8)7(9)4-5/h2-4H,1H3
InchiKey:	VISJRVXHPNMYRH-UHFFFAOYSA-N
Formula:	C7H6Cl2O
SMILES:	COc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	177.03
CAS:	36404-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-27.65	kJ/mol	Joback Method
hf	-137.92	kJ/mol	Joback Method
hfus	16.73	kJ/mol	Joback Method
hvap	45.96	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.002		Crippen Method
mcvol	116.080	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1271.00		NIST Webbook
rinpol	1310.90		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1307.50		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1310.90		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1899.00		NIST Webbook

ripol	1878.00		NIST Webbook
tb	493.48	K	Joback Method
tc	720.45	K	Joback Method
tf	302.18	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.95	J/mol×K	493.48	Joback Method
cpg	216.08	J/mol×K	531.31	Joback Method
cpg	224.74	J/mol×K	569.14	Joback Method
cpg	232.93	J/mol×K	606.96	Joback Method
cpg	240.65	J/mol×K	644.79	Joback Method
cpg	247.90	J/mol×K	682.62	Joback Method
cpg	254.69	J/mol×K	720.45	Joback Method
dvisc	0.0013457	Pa×s	302.18	Joback Method
dvisc	0.0008743	Pa×s	334.06	Joback Method
dvisc	0.0006124	Pa×s	365.95	Joback Method
dvisc	0.0004541	Pa×s	397.83	Joback Method
dvisc	0.0003521	Pa×s	429.71	Joback Method
dvisc	0.0002827	Pa×s	461.60	Joback Method
dvisc	0.0002335	Pa×s	493.48	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36404305&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
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