

Benzene, 1,2,4,5-tetrachloro-3-methoxy-

Other names:	Anisole, 2,3,5,6-tetrachloro- 2,3,5,6-Tetrachloroanisole 1,2,4,5-tetrachloro-3-methoxybenzene
Inchi:	InChI=1S/C7H4Cl4O/c1-12-7-5(10)3(8)2-4(9)6(7)11/h2H,1H3
InchiKey:	WMMFIDNWZNCBCT-UHFFFAOYSA-N
Formula:	C7H4Cl4O
SMILES:	COc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	245.92
CAS:	6936-40-9

Physical Properties

Property code	Value	Unit	Source
gf	-70.77	kJ/mol	Joback Method
hf	-192.34	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.309		Crippen Method
mcvol	140.560	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
ripol	1516.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	2021.00		NIST Webbook
ripol	2071.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2046.00		NIST Webbook
tb	578.30	K	Joback Method
tc	816.84	K	Joback Method
tf	387.06	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.24	J/molxK	578.30	Joback Method
cpg	277.88	J/molxK	777.08	Joback Method
cpg	272.20	J/molxK	737.33	Joback Method
cpg	266.09	J/molxK	697.57	Joback Method
cpg	259.55	J/molxK	657.81	Joback Method
cpg	252.60	J/molxK	618.06	Joback Method
cpg	283.12	J/molxK	816.84	Joback Method
dvisc	0.0002195	Paxs	578.30	Joback Method
dvisc	0.0002581	Paxs	546.43	Joback Method
dvisc	0.0003096	Paxs	514.55	Joback Method
dvisc	0.0003804	Paxs	482.68	Joback Method
dvisc	0.0004813	Paxs	450.81	Joback Method
dvisc	0.0006311	Paxs	418.93	Joback Method
dvisc	0.0008652	Paxs	387.06	Joback Method

Sources

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=C6936409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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