

Phenol, 2,3,5,6-tetrachloro-4-methoxy-

Other names:	p-Methoxytetrachlorophenol Drosophilin A Tetrachloro-p-methoxyphenol 2,3,5,6-Tetrachloro-4-methoxyphenol 4-Methoxy-2,3,5,6-tetrachlorophenol
Inchi:	InChI=1S/C7H4Cl4O2/c1-13-7-4(10)2(8)6(12)3(9)5(7)11/h12H,1H3
InchiKey:	XIWJLPHQDBDOAN-UHFFFAOYSA-N
Formula:	C7H4Cl4O2
SMILES:	COc1c(Cl)c(Cl)c(O)c(Cl)c1Cl
Mol. weight [g/mol]:	261.92
CAS:	484-67-3

Physical Properties

Property code	Value	Unit	Source
gf	-225.39	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	4.014		Crippen Method
mcvol	146.430	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	658.92	K	Joback Method
tc	906.45	K	Joback Method
tf	498.78	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.46	J/molxK	658.92	Joback Method
cpg	308.03	J/molxK	865.19	Joback Method
cpg	302.89	J/molxK	823.94	Joback Method
cpg	297.50	J/molxK	782.68	Joback Method

cpg	291.84	J/molxK	741.43	Joback Method
cpg	285.84	J/molxK	700.17	Joback Method
cpg	312.99	J/molxK	906.45	Joback Method
dvisc	0.0000252	Paxs	658.92	Joback Method
dvisc	0.0000329	Paxs	632.23	Joback Method
dvisc	0.0000438	Paxs	605.54	Joback Method
dvisc	0.0000599	Paxs	578.85	Joback Method
dvisc	0.0000845	Paxs	552.16	Joback Method
dvisc	0.0001234	Paxs	525.47	Joback Method
dvisc	0.0001877	Paxs	498.78	Joback Method

Sources

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=C484673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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