Chlorotrianisene

Other names:	Ethylene, chlorotris(p-methoxyphenyl)-
	Anisene
	Chlorotrianisine
	Chlorotris(p-methoxyphenyl)ethylene
	Chlortrianizen
	Clorestrolo
	Clorotrisin
	Hormonisene
	Khlortrianizen
	Merbentul
	Metace
	NSC-10108
	Rianil
	Tace
	Tri-p-anisylchloroethylene
	Tris(p-methoxyphenyl)chloroethylene
	Chloortrianisestrol
	Chlortrianisestrol
	Chlorestrolo
	1,1',1''-(1-Chloro-1-ethenyl-2-ylidene)-tris(4-methoxybenzene)
	Chlorotrianizen
	Chlorotrisin
	Chlortrianisen
	CTA
	Tace-fn
	Trianisestrol
	Benzene, 1,1',1''-(1-chloro-1-ethenyl-2-ylidene)tris(4-methoxy)-
	Tace (pharmaceutical)
Inchi:	InChI=1S/C23H21ClO3/c1-25-19-10-4-16(5-11-19)22(17-6-12-20(26-2)13-7-17)23(24)18
InchiKey:	BFPSDSIWYFKGBC-UHFFFAOYSA-N
Formula:	C23H21ClO3
SMILES:	COc1ccc(C(Cl)=C(c2ccc(OC)cc2)c2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	380.86
CAS:	569-57-3

Physical Properties

Property code	Value	Unit	Source

gf	187.31	kJ/mol	Joback Method
hf	-157.63	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.868		Crippen Method
mcvol	289.200	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
tb	929.23	K	Joback Method
tc	1180.24	K	Joback Method
tf	529.40	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.57	J/mol×K	929.23	Joback Method
cpg	864.87	J/mol×K	971.06	Joback Method
cpg	877.66	J/mol×K	1012.90	Joback Method
cpg	889.02	J/mol×K	1054.73	Joback Method
cpg	899.01	J/mol×K	1096.57	Joback Method
cpg	907.71	J/mol×K	1138.40	Joback Method
cpg	915.18	J/mol×K	1180.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C569573&Units=SI
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

Legend

cpg: Ideal gas heat capacity

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