Benzene, 1,1',1''-(1-chloro-1-ethenyl-2-ylidene)tris[4-methox

Other names: 1,1',1''-(1-Chloro-1-ethenyl-2-ylidene)-tris(4-methoxybenzene)
Anisene
Benzene, 1,1',1''-(1-chloro-1-ethenyl-2-ylidene)tris(4-methoxy)-
CTA
Chloortrianisestrol
Chlorestrolo
Chlorotrianisine
Chlorotrianizen
Chlorotris(p-methoxyphenyl)ethylene
Chlorotrisin
Chlortrianisen
Chlortrianisestrol
Chlortrianizen
Clorestrolo
Clorotrisin
Ethylene, chlorotris(p-methoxyphenyl)-
Hormonisene
Khlortrianizen
Merbentul
Metace
NSC-10108
Rianil
Tace
Tace (pharmaceutical)
Tace-fn
Tri-p-anisylchloroethylene
Trianisestrol
Tris(p-methoxyphenyl)chloroethylene

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]: 380.87

Physical Properties

Property code	Value	Unit	Source

hf	-162.03	kJ/mol	Cheméo Relay (1.0)
hfus	41.62	kJ/mol	Joback Method
hvap	120.76	kJ/mol	Cheméo Relay (1.0)
ie	7.24	eV	Cheméo Relay (1.0)
log10ws	-6.86		Cheméo Relay (1.0)
logp	5.868		Crippen Method
mcvol	289.200	ml/mol	McGowan Method
tb	728.14	K	Cheméo Relay (1.0)
tc	1015.10	K	Cheméo Relay (1.0)
tf	423.97	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C569573&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point