Clomiphene

Other names:	Clomifene
	Ethanamine, 2-[4-(2-chloro-1,2-diphenylethenyl)phenoxy]-N,N-diethyl-
	Triethylamine, 2-(p-(2-chloro-1,2-diphenylvinyl)phenoxy)-
	2-(4-(2-Chloro-1,2-diphenylethenyl)phenoxy)-N,N-diethylethanamine
	2-(p-(«beta»-Chloro-«alpha»-phenylstyryl)phenoxy)-triethylamine
	Cisclomiphene
	Clomiphene B
	1-(p-(«beta»-Diethylaminoethoxy)-phenyl)-1,2-diphenylchloroethylene
	2-[p-(2-Chloro-1,2-diphenylvinyl)phenoxy]triethylamine
Inchi:	InChI=1S/C26H28ClNO/c1-3-28(4-2)19-20-29-24-17-15-22(16-18-24)25(21-11-7-5-8-12-
InchiKey:	GKIRPKYJQBWNGO-QPLCGJKRSA-N
Formula:	C26H28ClNO
SMILES:	CCN(CC)CCOc1ccc(C(=C(Cl)c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]:	405.96
CAS:	911-45-5

Physical Properties

Property code	Value	Unit	Source
gf	552.61	kJ/mol	Joback Method
hf	135.36	kJ/mol	Joback Method
hfus	50.82	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.563		Crippen Method
mcvol	329.710	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2930.00		NIST Webbook
tb	955.51	K	Joback Method
tc	1198.20	K	Joback Method
tf	526.18	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.81	J/mol×K	955.51	Joback Method
cpg	1034.18	J/mol×K	995.96	Joback Method
cpg	1049.40	J/mol×K	1036.41	Joback Method
cpg	1063.61	J/mol×K	1076.85	Joback Method
cpg	1076.96	J/mol×K	1117.30	Joback Method
cpg	1089.63	J/mol×K	1157.75	Joback Method
cpg	1101.75	J/mol×K	1198.20	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=C911455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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