Tamoxifen

Other names:	Ethanamine, 2-[4-(1,2-diphenyl-1-butenyl)phenoxy]-N,N-dimethyl-, (Z)- Ethylamine, N,N-dimethyl-2-(p-(1,2-diphenyl-1-butenyl)phenoxy)-, (Z)- cis-1-(p-(2-(N,N-Dimethylamino)ethoxy)phenyl)-1,2-diphenylbut-1-ene cis-N,N-Dimethyl-2-(p-(1,2-diphenyl-1-butenyl)phenoxy)ethylamine (Z)-2-(p-(1,2-Diphenyl-1-butenyl)-phenoxy)-N,N-dimethylethylamine ICI 46,474 Novadex Nolvadex (Z)-2-[p-(1,2-Diphenyl-1-butenyl)phenoxy]-N,N-dimethylethanamine Ethanamine, 2-[4-[(1Z)-1,2-diphenyl-1-buten-1-yl]phenoxy]-N,N-dimethyl- 2-[4-[(1Z)-1,2-diphenyl-1-buten-1-yl]phenoxy]-N,N-dimethylethanamine (tamoxifen)
Inchi:	InChI=1S/C26H29NO/c1-4-25(21-11-7-5-8-12-21)26(22-13-9-6-10-14-22)23-15-17-24(18
InchiKey:	NKANXQFJJICGDU-OCEACIFDSA-N
Formula:	C26H29NO
SMILES:	CCC(=C(c1ccccc1)c1ccc(OCCN(C)C)cc1)c1ccccc1
Mol. weight [g/mol]:	371.51
CAS:	10540-29-1

Physical Properties

Property code	Value	Unit	Source
gf	564.54	kJ/mol	Joback Method
hf	151.10	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.996		Crippen Method
mcvol	317.470	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
tb	918.08	K	Joback Method
tc	1157.78	K	Joback Method
tf	496.26	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.58	J/mol×K	1117.83	Joback Method
cpg	992.60	J/mol×K	918.08	Joback Method
cpg	1010.29	J/mol×K	958.03	Joback Method
cpg	1026.69	J/mol×K	997.98	Joback Method
cpg	1041.94	J/mol×K	1037.93	Joback Method
cpg	1056.19	J/mol×K	1077.88	Joback Method
cpg	1082.27	J/mol×K	1157.78	Joback Method
hfust	34.00	kJ/mol	371.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10540291&Units=SI

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
hfust: Enthalpy of fusion at a given temperature
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