Phenyltoloxamine

Other names:	Ethanamine, N,N-dimethyl-2-[2-(phenylmethyl)phenoxy]-
	Ethylamine, N,N-dimethyl-2-[(«alpha»-phenyl-o-tolyl)oxy]-
	o-Benzylphenyl 2-(dimethylamino)ethyl ether
	Antin
	Bistrimin
	Bristamin
	C 5581 H
	Fenoxadrin
	Histionex
	Phenoxadrin
	Phenoxadrine
	Phentoloxamine
	PRN
	2-(2-Benzylphenoxy)-N,N-dimethylethylamine
	2-[2-(Dimethylamino)ethoxy]diphenylmethane
	2-Benzylphenyl-«beta»-dimethylamino ethyl ether
	N,N-Dimethyl-2-(«alpha»-phenyl-o-toloxy)ethylamine
	N,N-Dimethyl-2-((«alpha»-phenyl-o-tolyl)oxy)ethylamine
	Phentoloxamin
Inchi:	InChI=1S/C17H21NO/c1-18(2)12-13-19-17-11-7-6-10-16(17)14-15-8-4-3-5-9-15/h3-11H,
InchiKey:	IZRPKIZLIFYYKR-UHFFFAOYSA-N
Formula:	C17H21NO
SMILES:	CN(C)CCOc1ccccc1Cc1ccccc1
Mol. weight [g/mol]:	255.35
CAS:	92-12-6

Physical Properties

Property code	Value	Unit	Source
gf	313.23	kJ/mol	Joback Method
hf	2.69	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	63.10	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.218		Crippen Method
mcvol	218.720	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1926.00		NIST Webbook

rinpol	1915.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	681.56	K	Joback Method
tc	901.89	K	Joback Method
tf	401.41	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.47	J/mol×K	681.56	Joback Method
cpg	609.79	J/mol×K	718.28	Joback Method
cpg	626.85	J/mol×K	755.00	Joback Method
cpg	642.71	J/mol×K	791.73	Joback Method
cpg	657.43	J/mol×K	828.45	Joback Method
cpg	671.07	J/mol×K	865.17	Joback Method
cpg	683.68	J/mol×K	901.89	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92126&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

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