Ethylamine, 2-[1-(p-chlorophenyl)-1-phenylethoxy]-N,N-dimeth

Other names: p-Chlor-«alpha»-methyl-diphenhydramin
2-(1-(p-Chlorophenyl)-1-phenylethoxy)-N,N-dimethylethylamine
«beta»-Dimethylamino-aethyl-(p-chlor-«alpha»-methylbenzhydryl)-aether
Chlorphenoxamine
2-[1-(4-Chlorophenyl)-1-phenylethoxy]-N,N-dimethylethanamine
Ethanamine, 2-[1-(4-chlorophenyl)-1-phenylethoxy]-N,N-dimethyl-
2-(1-(4-chlorophenyl)-1-phenylethoxy)-N,N-dimethylethylamine

Inchi: InChI=1S/C18H22ClNO/c1-18(21-14-13-20(2)3,15-7-5-4-6-8-15)16-9-11-17(19)12-10-16/

InchiKey: KKHPNPMTPORSQE-UHFFFAOYSA-N

Formula: C18H22ClNO

SMILES: CN(C)CCOC(C)(c1ccccc1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 303.83

CAS: 77-38-3

Physical Properties

Property code	Value	Unit	Source
gf	312.56	kJ/mol	Joback Method
hf	-42.44	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	68.42	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.182		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	738.64	K	Joback Method
tc	969.76	K	Joback Method
tf	445.02	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	677.90	J/mol×K	738.64	Joback Method
cpg	695.59	J/mol×K	777.16	Joback Method
cpg	711.91	J/mol×K	815.68	Joback Method
cpg	726.95	J/mol×K	854.20	Joback Method
cpg	740.83	J/mol×K	892.72	Joback Method
cpg	753.63	J/mol×K	931.24	Joback Method
cpg	765.47	J/mol×K	969.76	Joback Method

Sources

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=C77383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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