PHENOXYBENZAMINE

Other names: Benzenemethanamine, N-(2-chloroethyl)-N-(1-methyl-2-phenoxyethyl)-
Benzylamine, N-(2-chloroethyl)-N-(1-methyl-2-phenoxyethyl)-
Bensylyt
Benzylyt
Dibenylin
Dibenyline
Dibenzyline
688A
A 688
Bensylyte
2-(N-Benzyl-2-chloroethylamino)-1-phenoxypropane
Benzyl(2-chloroethyl)-(1-methyl-2-phenoxyethyl)amine
N-(2-Chloroethyl)-N-(1-methyl-2-phenoxyethyl)benzenemethanamine
N-(2-Chloroethyl)-N-(1-methyl-2-phenoxyethyl)benzylamine
NSC 37448
N-Phenoxyisopropyl-N-benzyl-«beta»-chloroethylamine

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

InchiKey: QZVCTJOXCFMACW-UHFFFAOYSA-N

Formula: C18H22ClNO

SMILES: CC(COc1ccccc1)N(CCCl)Cc1ccccc1

Mol. weight [g/mol]: 303.83

Physical Properties

Property code	Value	Unit	Source
hfus	35.34	kJ/mol	Joback Method
logp	4.195		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
rinpol	2205.00		NIST Webbook
rinpol	2233.00		NIST Webbook
rinpol	2233.00		NIST Webbook
tb	649.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.94	J/mol×K	736.45	Joback Method
cpg	694.53	J/mol×K	773.59	Joback Method
cpg	710.82	J/mol×K	810.73	Joback Method
cpg	725.87	J/mol×K	847.87	Joback Method
cpg	739.76	J/mol×K	885.01	Joback Method
cpg	752.58	J/mol×K	922.15	Joback Method
cpg	764.38	J/mol×K	959.29	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59961&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature