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
CAS:	59-96-1

Physical Properties

Property code	Value	Unit	Source
gf	316.91	kJ/mol	Joback Method
hf	-27.50	kJ/mol	Joback Method
hfus	35.34	kJ/mol	Joback Method
hvap	68.66	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.195		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2233.00		NIST Webbook
tb	736.45	K	Joback Method
tc	959.29	K	Joback Method

tf	415.08	K	Joback Method
vc	0.906	m3/kmol	Joback Method

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

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=C59961&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
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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