1-Methyl-2-phenoxyethylamine

Other names:	Ethylamine, 1-methyl-2-phenoxy- Ethylamine, methyl-2-phenoxy- «alpha»-Methyl-2-phenoxyethanamine Phenoxyisopropylamine 2-Phenoxy-1-methylethylamine 1-Phenoxy-2-propanamine 1-Phenoxy-2-propylamine 2-Amino-1-phenoxypropane 2-Propanamine, 1-phenoxy- C 1926 2-Phenoxyisopropylamine NSC 137777
Inchi:	InChI=1S/C9H13NO/c1-8(10)7-11-9-5-3-2-4-6-9/h2-6,8H,7,10H2,1H3
InchiKey:	IKYFHRVPKIFGMH-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	CC(N)COc1ccccc1
Mol. weight [g/mol]:	151.21
CAS:	35205-54-0

Physical Properties

Property code	Value	Unit	Source
gf	96.32	kJ/mol	Joback Method
hf	-96.27	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	50.57	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.413		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	526.51	K	Joback Method
tc	748.48	K	Joback Method
tf	308.10	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.50	J/mol×K	526.51	Joback Method
cpg	309.62	J/mol×K	563.50	Joback Method
cpg	322.91	J/mol×K	600.50	Joback Method
cpg	335.40	J/mol×K	637.49	Joback Method
cpg	347.11	J/mol×K	674.49	Joback Method
cpg	358.07	J/mol×K	711.48	Joback Method
cpg	368.29	J/mol×K	748.48	Joback Method

Sources

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=C35205540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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