Benzenamine, 3-phenoxy-

Other names:	m-Phenoxyaniline
	3-Aminodiphenyl ether
	m-Aminophenyl phenyl ether
	Aniline, m-phenoxy-
	3-Phenoxyaniline
Inchi:	InChI=1S/C12H11NO/c13-10-5-4-8-12(9-10)14-11-6-2-1-3-7-11/h1-9H,13H2
InchiKey:	UCSYVYFGMFODMY-UHFFFAOYSA-N
Formula:	C12H11NO
SMILES:	Nc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	185.22
CAS:	3586-12-7

Physical Properties

Property code	Value	Unit	Source
gf	226.80	kJ/mol	Joback Method
hf	72.15	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	60.57	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	3.061		Crippen Method
mcvol	148.270	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	588.00	K	NIST Webbook
tb	602.70	K	NIST Webbook
tb	588.20	K	NIST Webbook
tc	881.74	K	Joback Method
tf	310.00	K	NIST Webbook
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.85	J/mol×K	627.25	Joback Method
cpg	374.56	J/mol×K	669.67	Joback Method

cpg	388.09	J/mol×K	712.08	Joback Method
cpg	400.50	J/mol×K	754.50	Joback Method
cpg	411.83	J/mol×K	796.91	Joback Method
cpg	422.13	J/mol×K	839.33	Joback Method
cpg	431.47	J/mol×K	881.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.50 ± 1.50	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3586127&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume