3-Benzyloxyaniline

Other names: Benzenamine, 3-(phenylmethoxy)-
3-Aminophenyl benzyl ether
Inchi: InChI=1S/C13H13NO/c14-12-7-4-8-13(9-12)15-10-11-5-2-1-3-6-11/h1-9H,10,14H2
InchiKey: IGPFOKFDBICQMC-UHFFFAOYSA-N
Formula: C13H13NO
SMILES: Nc1cccc(OCc2ccccc2)c1
Mol. weight [g/mol]: 199.25
CAS: 1484-26-0

Physical Properties

Property code	Value	Unit	Source
gf	235.22	kJ/mol	Joback Method
hf	51.51	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-3.33		Crippen Method
logp	2.848		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	650.13	K	Joback Method
tc	898.85	K	Joback Method
tf	407.12	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.06	J/mol×K	650.13	Joback Method
cpg	424.41	J/mol×K	691.58	Joback Method
cpg	438.54	J/mol×K	733.04	Joback Method
cpg	451.53	J/mol×K	774.49	Joback Method
cpg	463.43	J/mol×K	815.94	Joback Method
cpg	474.28	J/mol×K	857.39	Joback Method

cpg	484.14	J/mol×K	898.85	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=C1484260&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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume