Benzylamine, n-(o-nitrophenyl)-

Inchi: InChI=1S/C13H12N2O2/c16-15(17)13-9-5-4-8-12(13)14-10-11-6-2-1-3-7-11/h1-9,14H,10
InchiKey: LAOUKNRSKBRAMQ-UHFFFAOYSA-N
Formula: C13H12N2O2
SMILES: O=[N+]([O-])c1ccccc1NCc1ccccc1
Mol. weight [g/mol]: 228.25
CAS: 5729-06-6

Physical Properties

Property code	Value	Unit	Source
gf	398.71	kJ/mol	Joback Method
hf	192.65	kJ/mol	Joback Method
hfus	33.58	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.207		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	757.19	K	Joback Method
tc	1020.62	K	Joback Method
tf	497.90	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.05	J/mol×K	757.19	Joback Method
cpg	486.47	J/mol×K	801.09	Joback Method
cpg	498.63	J/mol×K	845.00	Joback Method
cpg	509.64	J/mol×K	888.90	Joback Method
cpg	519.60	J/mol×K	932.81	Joback Method
cpg	528.61	J/mol×K	976.71	Joback Method
cpg	536.77	J/mol×K	1020.62	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=C5729066&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume