Benzene, 1-nitro-4-(2-phenylethyl)-

Other names: Bibenzyl, 4-nitro-
p-Nitrobibenzyl
4-Nitrobibenzyl
Inchi: InChI=1S/C14H13NO2/c16-15(17)14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-5,8-11H,6-
InchiKey: FCVDHPQXWWONCH-UHFFFAOYSA-N
Formula: C14H13NO2
SMILES: O=[N+]([O-])c1ccc(CCc2ccccc2)cc1
Mol. weight [g/mol]: 227.26
CAS: 14310-29-3

Physical Properties

Property code	Value	Unit	Source
gf	317.74	kJ/mol	Joback Method
hf	118.54	kJ/mol	Joback Method
hfus	31.07	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
ie	9.17 ± 0.05	eV	NIST Webbook
ie	8.90 ± 0.10	eV	NIST Webbook
log10ws	-4.54		Crippen Method
logp	3.380		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
tb	729.90	K	Joback Method
tc	991.74	K	Joback Method
tf	456.51	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.51	J/mol×K	729.90	Joback Method
cpg	490.22	J/mol×K	773.54	Joback Method
cpg	503.62	J/mol×K	817.18	Joback Method
cpg	515.81	J/mol×K	860.82	Joback Method

cpg	526.88	J/mol×K	904.46	Joback Method
cpg	536.95	J/mol×K	948.10	Joback Method
cpg	546.10	J/mol×K	991.74	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=C14310293&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
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