

Benzene, 1-nitro-4-(phenylmethoxy)-

Other names:	Benzyl p-nitrophenyl ether Ether, benzyl p-nitrophenyl 4-Benzyloxynitrobenzene Nitrobenzene, 4-(phenylmethoxy)- Benzyl 4-nitrophenyl ether p-(benzyloxy)nitrobenzene
Inchi:	InChI=1S/C13H11NO3/c15-14(16)12-6-8-13(9-7-12)17-10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey:	YOVUXLHIVNBVKO-UHFFFAOYSA-N
Formula:	C13H11NO3
SMILES:	O=[N+](O)c1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	229.23
CAS:	1145-76-2

Physical Properties

Property code	Value	Unit	Source
gf	204.32	kJ/mol	Joback Method
hf	6.96	kJ/mol	Joback Method
hfus	29.67	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-4.35		Crippen Method
logp	3.174		Crippen Method
mvol	169.800	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	729.44	K	Joback Method
tc	992.73	K	Joback Method
tf	467.47	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.48	J/molxK	729.44	Joback Method
cpg	462.29	J/molxK	773.32	Joback Method

cpg	474.81	J/mol×K	817.20	Joback Method
cpg	486.12	J/mol×K	861.09	Joback Method
cpg	496.27	J/mol×K	904.97	Joback Method
cpg	505.35	J/mol×K	948.85	Joback Method
cpg	513.41	J/mol×K	992.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1145762&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
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

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