Ether, bis(m-nitrobenzyl)-

Inchi: InChI=1S/C14H12N2O5/c17-15(18)13-5-1-3-11(7-13)9-21-10-12-4-2-6-14(8-12)16(19)20
InchiKey: LDDKBZYKNBNGSA-UHFFFAOYSA-N
Formula: C14H12N2O5
SMILES: O=[N+]([O-])c1cccc(COCc2cccc([N+](=O)[O-])c2)c1
Mol. weight [g/mol]: 288.26
CAS: 27183-43-3

Physical Properties

Property code	Value	Unit	Source
gf	238.66	kJ/mol	Joback Method
hf	-35.91	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	88.23	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.220		Crippen Method
mcvol	201.310	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	909.14	K	Joback Method
tc	1181.60	K	Joback Method
tf	634.87	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.43	J/mol×K	909.14	Joback Method
cpg	600.06	J/mol×K	954.55	Joback Method
cpg	609.42	J/mol×K	999.96	Joback Method
cpg	617.60	J/mol×K	1045.37	Joback Method
cpg	624.68	J/mol×K	1090.78	Joback Method
cpg	630.72	J/mol×K	1136.19	Joback Method
cpg	635.82	J/mol×K	1181.60	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=C27183433&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
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