N-(2-Phenylethyl)aminoacetaldehyde diethyl acetal

Inchi: InChI=1S/C14H23NO2/c1-3-16-14(17-4-2)12-15-11-10-13-8-6-5-7-9-13/h5-9,14-15H,3-4
InchiKey: IZISGBNIQIHBHI-UHFFFAOYSA-N
Formula: C14H23NO2
SMILES: CCOC(CNCCc1ccccc1)OCC
Mol. weight [g/mol]: 237.34
CAS: 94508-09-5

Physical Properties

Property code	Value	Unit	Source
gf	56.36	kJ/mol	Joback Method
hf	-312.01	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	59.90	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.218		Crippen Method
mcvol	206.080	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
tb	640.97	K	Joback Method
tc	836.58	K	Joback Method
tf	356.08	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.75	J/mol×K	640.97	Joback Method
cpg	572.99	J/mol×K	673.57	Joback Method
cpg	589.31	J/mol×K	706.17	Joback Method
cpg	604.72	J/mol×K	738.77	Joback Method
cpg	619.24	J/mol×K	771.38	Joback Method
cpg	632.89	J/mol×K	803.98	Joback Method
cpg	645.68	J/mol×K	836.58	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=C94508095&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