(2-Dimethylamino)ethyl-1,2-diphenylethyl ether (from Bibenzonium bromide)

Inchi: InChI=1S/C18H23NO/c1-19(2)13-14-20-18(17-11-7-4-8-12-17)15-16-9-5-3-6-10-16/h3-12

InchiKey: LVKVUFDVHFLQDJ-UHFFFAOYSA-N

Formula: C18H23NO

SMILES: CN(C)CCOC(Cc1ccccc1)c1ccccc1

Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	328.84	kJ/mol	Joback Method
hf	-11.76	kJ/mol	Joback Method
hfus	31.14	kJ/mol	Joback Method
hvap	64.28	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.549		Crippen Method
mcvol	232.810	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1923.00		NIST Webbook
tb	699.02	K	Joback Method
tc	918.94	K	Joback Method
tf	385.16	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.07	J/mol×K	699.02	Joback Method
cpg	666.13	J/mol×K	735.67	Joback Method
cpg	683.85	J/mol×K	772.33	Joback Method
cpg	700.29	J/mol×K	808.98	Joback Method
cpg	715.52	J/mol×K	845.63	Joback Method
cpg	729.61	J/mol×K	882.28	Joback Method
cpg	742.63	J/mol×K	918.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R489197&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume