N,N-di-(1-Phenylethyl)amine, diastereomer # 1

Inchi: InChI=1S/C16H19N/c1-13(15-9-5-3-6-10-15)17-14(2)16-11-7-4-8-12-16/h3-14,17H,1-2H
InchiKey: NXLACVVNHYIYJN-UHFFFAOYSA-N
Formula: C16H19N
SMILES: CC(NC(C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 225.33

Physical Properties

Property code	Value	Unit	Source
gf	393.17	kJ/mol	Joback Method
hf	142.40	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.098		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
tb	668.13	K	Joback Method
tc	905.79	K	Joback Method
tf	345.58	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.61	J/mol×K	668.13	Joback Method
cpg	547.15	J/mol×K	707.74	Joback Method
cpg	564.27	J/mol×K	747.35	Joback Method
cpg	580.04	J/mol×K	786.96	Joback Method
cpg	594.57	J/mol×K	826.57	Joback Method
cpg	607.94	J/mol×K	866.18	Joback Method
cpg	620.23	J/mol×K	905.79	Joback Method

Sources

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=R636452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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