BENZENEPROPANAMINE, N,N,4-TRIMETHYL-.GAMMA.-PHENYL-

Other names: Benzenepropanamine, N,N,4-trimethyl-«gamma»-phenyl-
N,N-Dimethyl-3-phenyl-3-p-tolylpropylamine
N,N-Dimethyl-3-phenyl-3-p-tolylpropamine
Tolpropamide

Inchi: InChI=1S/C18H23N/c1-15-9-11-17(12-10-15)18(13-14-19(2)3)16-7-5-4-6-8-16/h4-12,18H

InchiKey: CINROOONPHQHPO-UHFFFAOYSA-N

Formula: C18H23N

SMILES: Cc1ccc(C(CCN(C)C)c2ccccc2)cc1

Mol. weight [g/mol]: 253.39

Physical Properties

Property code	Value	Unit	Source
hfus	29.57	kJ/mol	Joback Method
hvap	85.31	kJ/mol	Cheméo Relay (1.0)
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	4.079		Crippen Method
mcvol	226.940	ml/mol	McGowan Method
rinpol	1900.00		NIST Webbook
tb	611.72	K	Cheméo Relay (1.0)
tf	312.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.89	J/mol×K	681.58	Joback Method
cpg	637.41	J/mol×K	718.82	Joback Method
cpg	655.56	J/mol×K	756.06	Joback Method
cpg	672.42	J/mol×K	793.31	Joback Method
cpg	688.09	J/mol×K	830.55	Joback Method
cpg	702.63	J/mol×K	867.79	Joback Method
cpg	716.13	J/mol×K	905.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5632440&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point