Terodiline

Other names: Benzenepropanamine, N-(1,1-dimethylethyl)-«alpha»-methyl-«gamma»-phenyl-
Propylamine, N-tert-butyl-1-methyl-3,3-diphenyl-
Bicor
N-tert-Butyl-1-methyl-3,3-diphenylpropylamine
Inchi: InChI=1S/C20H27N/c1-16(21-20(2,3)4)15-19(17-11-7-5-8-12-17)18-13-9-6-10-14-18/h5-
InchiKey: UISARWKNNNHPGI-UHFFFAOYSA-N
Formula: C20H27N
SMILES: CC(CC(c1ccccc1)c1ccccc1)NC(C)(C)C
Mol. weight [g/mol]: 281.44
CAS: 15793-40-5

Physical Properties

Property code	Value	Unit	Source
gf	429.69	kJ/mol	Joback Method
hf	51.09	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.985		Crippen Method
mcvol	255.120	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	1908.00		NIST Webbook
tb	756.42	K	Joback Method
tc	988.78	K	Joback Method
tf	393.08	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.43	J/mol×K	756.42	Joback Method
cpg	771.13	J/mol×K	795.15	Joback Method
cpg	789.34	J/mol×K	833.87	Joback Method
cpg	806.18	J/mol×K	872.60	Joback Method

cpg	821.79	J/mol×K	911.33	Joback Method
cpg	836.28	J/mol×K	950.05	Joback Method
cpg	849.79	J/mol×K	988.78	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=C15793405&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume