Benzenepropanamine, N,N,.alpha.-trimethyl-.gamma.-phenyl-

Other names: Benzenepropanamine, N,N,«alpha»-trimethyl-«gamma»-phenyl-
Propylamine, N,N,1-trimethyl-3,3-diphenyl-
N,N,«alpha»Trimethyl-«gamma»-phenylbenzenepropanamine
N,N-Dimethyl-4,4-diphenyl-2-butanamine
1,1-Diphenylbutane, 3-dimethylamino
2-Butanamine, N,N-dimethyl, 4,4-diphenyl

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

InchiKey: NSHMKXVHJBBKTN-UHFFFAOYSA-N

Formula: C18H23N

SMILES: CC(CC(c1ccccc1)c1ccccc1)N(C)C

Mol. weight [g/mol]: 253.39

Physical Properties

Property code	Value	Unit	Source
af	0.4871		Cheméo Relay (1.0)
gf	431.40	kJ/mol	Joback Method
hf	149.70	kJ/mol	Cheméo Relay (1.0)
hfus	26.43	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Cheméo Relay (1.0)
ie	7.86	eV	Cheméo Relay (1.0)
log10ws	-3.24		Cheméo Relay (1.0)
logp	4.159		Crippen Method
mcvol	226.940	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	595.77	K	Cheméo Relay (1.0)
tc	837.30	K	Cheméo Relay (1.0)
tf	289.03	K	Cheméo Relay (1.0)
vc	0.807	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	618.60	J/mol×K	676.16	Joback Method
cpg	638.74	J/mol×K	713.99	Joback Method
cpg	657.41	J/mol×K	751.82	Joback Method
cpg	674.70	J/mol×K	789.64	Joback Method
cpg	690.70	J/mol×K	827.47	Joback Method
cpg	705.52	J/mol×K	865.30	Joback Method
cpg	719.23	J/mol×K	903.13	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13957556&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

Legend

af: Acentric Factor
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
ie: Ionization energy
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

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