1,2-Diphenylethylamine

Other names: 1-Amino-1,2-diphenylethane
Benzeneethanamine, «alpha»-phenyl-
Phenethylamine, «alpha»-phenyl-
«alpha»-Benzylbenzylamine
«alpha»-Phenylphenethylamine
Inchi: InChI=1S/C14H15N/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10,14H,11,15H2
InchiKey: DTGGNTMERRTPLR-UHFFFAOYSA-N
Formula: C14H15N
SMILES: NC(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 197.28
CAS: 25611-78-3

Physical Properties

Property code	Value	Unit	Source
gf	355.83	kJ/mol	Joback Method
hf	169.28	kJ/mol	Joback Method
hfus	21.77	kJ/mol	Joback Method
hvap	61.56	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.929		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	645.17	K	Joback Method
tc	896.97	K	Joback Method
tf	368.64	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.40	J/mol×K	645.17	Joback Method
cpg	452.37	J/mol×K	687.14	Joback Method

cpg	467.94	J/mol×K	729.10	Joback Method
cpg	482.19	J/mol×K	771.07	Joback Method
cpg	495.23	J/mol×K	813.04	Joback Method
cpg	507.15	J/mol×K	855.01	Joback Method
cpg	518.04	J/mol×K	896.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	583.70	K	100.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25611783&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume