Benzenemethanamine, N,N-bis(phenylmethyl)-

Other names: (N,N-dibenzylaminomethyl)benzene
N,N,N-tribenzylamine
tribenzylamine
Inchi: InChI=1S/C21H21N/c1-4-10-19(11-5-1)16-22(17-20-12-6-2-7-13-20)18-21-14-8-3-9-15-2
InchiKey: MXHTZQSKTCCMFG-UHFFFAOYSA-N
Formula: C21H21N
SMILES: c1ccc(CN(Cc2ccccc2)Cc2ccccc2)cc1
Mol. weight [g/mol]: 287.40
CAS: 620-40-6

Physical Properties

Property code	Value	Unit	Source
chs	-11406.00 ± 11.00	kJ/mol	NIST Webbook
chs	-11557.00	kJ/mol	NIST Webbook
gf	573.95	kJ/mol	Joback Method
hf	300.35	kJ/mol	Joback Method
hfs	141.00 ± 11.00	kJ/mol	NIST Webbook
hfs	240.00	kJ/mol	NIST Webbook
hfus	35.29	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.889		Crippen Method
mcvol	245.450	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2271.00		NIST Webbook
ripol	3035.00		NIST Webbook
ripol	3035.00		NIST Webbook
tb	772.36	K	Joback Method
tc	1019.27	K	Joback Method
tf	438.16	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.23	J/mol×K	772.36	Joback Method
cpg	718.76	J/mol×K	813.51	Joback Method
cpg	735.71	J/mol×K	854.66	Joback Method
cpg	751.25	J/mol×K	895.82	Joback Method
cpg	765.50	J/mol×K	936.97	Joback Method
cpg	778.62	J/mol×K	978.12	Joback Method
cpg	790.77	J/mol×K	1019.27	Joback Method
hvapt	92.40	kJ/mol	298.00	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	1.70	NIST Webbook

Sources

Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15: https://www.doi.org/10.1021/je500358r

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=C620406&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	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