3-Methyldiphenylamine

Other names: Benzenamine, 3-methyl-N-phenyl-
N-phenyl-m-toluidine
3-methyl-N-phenylaniline
Inchi: InChI=1S/C13H13N/c1-11-6-5-9-13(10-11)14-12-7-3-2-4-8-12/h2-10,14H,1H3
InchiKey: TWPMMLHBHPYSMT-UHFFFAOYSA-N
Formula: C13H13N
SMILES: Cc1cccc(Nc2ccccc2)c1
Mol. weight [g/mol]: 183.25
CAS: 1205-64-7

Physical Properties

Property code	Value	Unit	Source
gf	363.16	kJ/mol	Joback Method
hf	203.41	kJ/mol	Joback Method
hfus	22.22	kJ/mol	Joback Method
hvap	56.18	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.739		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	605.35	K	Joback Method
tc	849.03	K	Joback Method
tf	354.29	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.27	J/mol×K	605.35	Joback Method
cpg	390.48	J/mol×K	645.96	Joback Method
cpg	405.44	J/mol×K	686.58	Joback Method
cpg	419.22	J/mol×K	727.19	Joback Method
cpg	431.91	J/mol×K	767.80	Joback Method
cpg	443.56	J/mol×K	808.41	Joback Method

cpg	454.25	J/mol×K	849.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1205647&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume