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

Physical Properties

Property code	Value	Unit	Source
af	0.5063		Cheméo Relay (1.0)
gf	363.16	kJ/mol	Joback Method
hf	162.96	kJ/mol	Cheméo Relay (1.0)
hfus	22.22	kJ/mol	Joback Method
hvap	77.30	kJ/mol	Cheméo Relay (1.0)
ie	7.31	eV	Cheméo Relay (1.0)
log10ws	-3.99		Cheméo Relay (1.0)
logp	3.739		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	584.82	K	Cheméo Relay (1.0)
tc	884.24	K	Cheméo Relay (1.0)
tf	300.34	K	Cheméo Relay (1.0)
vc	0.570	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1205647&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume