

N,N-di-p-tolyl-p-toluidine

Other names: 4-methyl-N,N-bis(4-methylphenyl)benzenamine

tri(4-methylphenyl)amine

tri-tolylamine

Inchi: InChI=1S/C21H21N/c1-16-4-10-19(11-5-16)22(20-12-6-17(2)7-13-20)21-14-8-18(3)9-15-

InchiKey: YXYUIABODWXVIK-UHFFFAOYSA-N

Formula: C₂₁H₂₁N

SMILES: Cc1ccc(N(c2ccc(C)cc2)c2ccc(C)cc2)cc1

Mol. weight [g/mol]: 287.40

CAS: 1159-53-1

Physical Properties

Property code	Value	Unit	Source
gf	545.06	kJ/mol	Joback Method
hf	265.94	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	73.20	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.082		Crippen Method
mcvol	245.450	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
tb	787.30	K	Joback Method
tc	1036.42	K	Joback Method
tf	388.74	K	Measurement and Prediction of Solubility of Four Arylamine Molecules in Benzene, Hexane, and Methanol
vc	0.905	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.56	J/mol×K	994.90	Joback Method
cpg	697.76	J/mol×K	787.30	Joback Method
cpg	715.87	J/mol×K	828.82	Joback Method

cpg	732.48	J/mol×K	870.34	Joback Method
cpg	747.72	J/mol×K	911.86	Joback Method
cpg	761.71	J/mol×K	953.38	Joback Method
cpg	786.40	J/mol×K	1036.42	Joback Method
hfust	19.95	kJ/mol	388.80	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Prediction of Solubility of Four Arylamine Molecules in Benzene, Hexane, and Methanol:	https://www.doi.org/10.1021/je0495785
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=C1159531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hfust:	Enthalpy of fusion at a given temperature
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

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