

N-benzyl-p-toluidine

Other names:	N-Benzyl-4-toluidine N-Benzyl-N-(4-methylphenyl)amine N-Benzyl-p-toluidine NSC 8084
Inchi:	InChI=1S/C14H15N/c1-12-7-9-14(10-8-12)15-11-13-5-3-2-4-6-13/h2-10,15H,11H2,1H3
InchiKey:	KEVOWRWHMCBERP-UHFFFAOYSA-N
Formula:	C14H15N
SMILES:	Cc1ccc(NCc2ccccc2)cc1
Mol. weight [g/mol]:	197.28
CAS:	500007-41-0

Physical Properties

Property code	Value	Unit	Source
af	0.5248		Cheméo Relay (1.0)
gf	371.58	kJ/mol	Joback Method
hf	169.42	kJ/mol	Cheméo Relay (1.0)
hfus	24.81	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Cheméo Relay (1.0)
ie	7.46	eV	Cheméo Relay (1.0)
log10ws	-3.87		Cheméo Relay (1.0)
logp	3.607		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	592.15 ± 3.00	K	NIST Webbook
tc	856.75	K	Cheméo Relay (1.0)
tf	326.00	K	Cheméo Relay (1.0)
vc	0.625	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.81	J/mol×K	628.23	Joback Method
cpg	440.56	J/mol×K	667.98	Joback Method
cpg	456.06	J/mol×K	707.73	Joback Method

cpg	470.37	J/mol×K	747.49	Joback Method
cpg	483.58	J/mol×K	787.24	Joback Method
cpg	495.75	J/mol×K	826.99	Joback Method
cpg	506.95	J/mol×K	866.74	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C500007410&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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