

N,N-Dimethylbenzenamine,2,4-di-t-butyl

Inchi:	InChI=1S/C16H27N/c1-15(2,3)12-9-10-14(17(7)8)13(11-12)16(4,5)6/h9-11H,1-8H3
InchiKey:	CQRQHMIMTXPFQJ-UHFFFAOYSA-N
Formula:	C16H27N
SMILES:	CN(C)c1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]:	233.39
CAS:	2909-76-4

Physical Properties

Property code	Value	Unit	Source
affp	973.30	kJ/mol	NIST Webbook
basg	942.40	kJ/mol	NIST Webbook
gf	293.45	kJ/mol	Joback Method
hf	-109.95	kJ/mol	Joback Method
hfus	18.65	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.348		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
tb	608.10	K	Joback Method
tc	818.57	K	Joback Method
tf	358.85	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.98	J/mol×K	608.10	Joback Method
cpg	610.85	J/mol×K	643.18	Joback Method
cpg	630.36	J/mol×K	678.26	Joback Method
cpg	648.60	J/mol×K	713.34	Joback Method
cpg	665.66	J/mol×K	748.42	Joback Method
cpg	681.63	J/mol×K	783.50	Joback Method
cpg	696.58	J/mol×K	818.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2909764&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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