

1-Naphthylamine, 2-tert-butyl-

Inchi:	InChI=1S/C14H17N/c1-14(2,3)12-9-8-10-6-4-5-7-11(10)13(12)15/h4-9H,15H2,1-3H3
InchiKey:	RCDMTTAHFWYLAA-UHFFFAOYSA-N
Formula:	C14H17N
SMILES:	CC(C)(C)c1ccc2ccccc2c1N
Mol. weight [g/mol]:	199.29
CAS:	110014-56-7

Physical Properties

Property code	Value	Unit	Source
gf	336.09	kJ/mol	Joback Method
hf	97.41	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	61.34	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.720		Crippen Method
mcvol	174.880	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	644.64	K	Joback Method
tc	889.01	K	Joback Method
tf	417.38	K	Joback Method
vc	0.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.29	J/mol×K	644.64	Joback Method
cpg	471.54	J/mol×K	685.37	Joback Method
cpg	486.54	J/mol×K	726.10	Joback Method
cpg	500.39	J/mol×K	766.83	Joback Method
cpg	513.22	J/mol×K	807.56	Joback Method
cpg	525.15	J/mol×K	848.28	Joback Method
cpg	536.29	J/mol×K	889.01	Joback Method

Sources

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=C110014567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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