Benzenamine, 2,4,6-tris(1,1-dimethylethyl)-

Other names:	2,4,6-tri-tert-Butylaniline
	2,4,6-tri-t-Butylaniline
	Aniline, tri-tert-butyl-
	Aniline, 2,4,6-tri-tert-butyl-
Inchi:	InChI=1S/C18H31N/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11H,19H
InchiKey:	REJGDSCBQPJPQT-UHFFFAOYSA-N
Formula:	C18H31N
SMILES:	CC(C)(C)c1cc(C(C)(C)C)c(N)c(C(C)(C)C)c1
Mol. weight [g/mol]:	261.45
CAS:	961-38-6

Physical Properties

Property code	Value	Unit	Source
gf	259.17	kJ/mol	Joback Method
hf	-205.19	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hsub	92.50 ± 1.10	kJ/mol	NIST Webbook
hvap	66.68	kJ/mol	Joback Method
ie	7.30	eV	NIST Webbook
ie	6.90	eV	NIST Webbook
log10ws	-5.05		Crippen Method
logp	5.161		Crippen Method
mcvol	250.700	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
tb	715.70	K	Joback Method
tc	941.27	K	Joback Method
tf	447.12	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.39	J/mol×K	715.70	Joback Method
cpg	756.58	J/mol×K	753.30	Joback Method

cpg	775.40	J/mol×K	790.89	Joback Method
cpg	792.98	J/mol×K	828.49	Joback Method
cpg	809.43	J/mol×K	866.08	Joback Method
cpg	824.87	J/mol×K	903.68	Joback Method
cpg	839.43	J/mol×K	941.27	Joback Method
hfust	19.38	kJ/mol	426.40	NIST Webbook

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=C961386&Units=SI

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
hsub:	Enthalpy of sublimation 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