

Aniline, 2-methyl-4,6-di-tert-butyl-

Inchi:	InChI=1S/C15H25N/c1-10-8-11(14(2,3)4)9-12(13(10)16)15(5,6)7/h8-9H,16H2,1-7H3
InchiKey:	KOENVNBHHIFQKL-UHFFFAOYSA-N
Formula:	C15H25N
SMILES:	Cc1cc(C(C)(C)C)cc(C(C)(C)C)c1N
Mol. weight [g/mol]:	219.37
CAS:	35532-73-1

Physical Properties

Property code	Value	Unit	Source
gf	231.07	kJ/mol	Joback Method
hf	-134.52	kJ/mol	Joback Method
hfus	17.85	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.172		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
tb	650.29	K	Joback Method
tc	875.75	K	Joback Method
tf	410.89	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.74	J/mol×K	650.29	Joback Method
cpg	588.57	J/mol×K	687.87	Joback Method
cpg	606.14	J/mol×K	725.44	Joback Method
cpg	622.53	J/mol×K	763.02	Joback Method
cpg	637.84	J/mol×K	800.60	Joback Method
cpg	652.15	J/mol×K	838.18	Joback Method
cpg	665.55	J/mol×K	875.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C35532731&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
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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