

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

Inchi:	InChI=1S/C15H25N/c1-14(2,3)11-8-9-13(16-7)12(10-11)15(4,5)6/h8-10,16H,1-7H3
InchiKey:	CRZSQVTUTVJLNH-UHFFFAOYSA-N
Formula:	C15H25N
SMILES:	CNc1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]:	219.37
CAS:	26461-68-7

Physical Properties

Property code	Value	Unit	Source
gf	263.64	kJ/mol	Joback Method
hf	-103.37	kJ/mol	Joback Method
hfus	18.14	kJ/mol	Joback Method
hvap	56.43	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	4.323		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
tb	622.95	K	Joback Method
tc	839.49	K	Joback Method
tf	367.77	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.04	J/molxK	622.95	Joback Method
cpg	576.49	J/molxK	659.04	Joback Method
cpg	594.65	J/molxK	695.13	Joback Method
cpg	611.61	J/molxK	731.22	Joback Method
cpg	627.45	J/molxK	767.31	Joback Method
cpg	642.26	J/molxK	803.40	Joback Method
cpg	656.12	J/molxK	839.49	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=C26461687&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
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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