

Aniline, 4-tert-butyl-2,6-diethyl-

Inchi:	InChI=1S/C14H23N/c1-6-10-8-12(14(3,4)5)9-11(7-2)13(10)15/h8-9H,6-7,15H2,1-5H3
InchiKey:	DXFBXESOGGKUEG-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCc1cc(C(C)(C)C)cc(CC)c1N
Mol. weight [g/mol]:	205.34
CAS:	67330-60-3

Physical Properties

Property code	Value	Unit	Source
gf	219.81	kJ/mol	Joback Method
hf	-105.13	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	60.36	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.691		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
tb	630.64	K	Joback Method
tc	847.50	K	Joback Method
tf	397.20	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.42	J/molxK	630.64	Joback Method
cpg	532.02	J/molxK	666.78	Joback Method
cpg	548.57	J/molxK	702.93	Joback Method
cpg	564.11	J/molxK	739.07	Joback Method
cpg	578.69	J/molxK	775.21	Joback Method
cpg	592.39	J/molxK	811.35	Joback Method
cpg	605.24	J/molxK	847.50	Joback Method

Sources

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=C67330603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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