

Aniline, 2-methyl-4-(1',1',3',3'-tetramethylbutyl)-

Inchi:	InChI=1S/C15H25N/c1-11-9-12(7-8-13(11)16)15(5,6)10-14(2,3)4/h7-9H,10,16H2,1-6H3
InchiKey:	IYHTUEGIFDQRBA-UHFFFAOYSA-N
Formula:	C15H25N
SMILES:	<chem>Cc1cc(C(C)(C)CC(C)(C)C)ccc1N</chem>
Mol. weight [g/mol]:	219.37

Physical Properties

Property code	Value	Unit	Source
gf	240.70	kJ/mol	Joback Method
hf	-123.05	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.291		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	645.31	K	Joback Method
tc	869.88	K	Joback Method
tf	398.37	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.00	J/molxK	645.31	Joback Method
cpg	589.06	J/molxK	682.74	Joback Method
cpg	606.81	J/molxK	720.17	Joback Method
cpg	623.35	J/molxK	757.59	Joback Method
cpg	638.76	J/molxK	795.02	Joback Method
cpg	653.16	J/molxK	832.45	Joback Method
cpg	666.62	J/molxK	869.88	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=B6009276&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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