

Aniline, 4-tert-butyl-n-(1,3-dimethylbutyl)-

Inchi:	InChI=1S/C16H27N/c1-12(2)11-13(3)17-15-9-7-14(8-10-15)16(4,5)6/h7-10,12-13,17H,11
InchiKey:	FMRJPZKPQMPPAA-UHFFFAOYSA-N
Formula:	C16H27N
SMILES:	CC(C)CC(C)Nc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	233.39

Physical Properties

Property code	Value	Unit	Source
gf	273.97	kJ/mol	Joback Method
hf	-114.35	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	58.51	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.831		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
tb	643.20	K	Joback Method
tc	851.92	K	Joback Method
tf	334.10	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.63	J/molxK	643.20	Joback Method
cpg	628.48	J/molxK	677.99	Joback Method
cpg	647.10	J/molxK	712.77	Joback Method
cpg	664.56	J/molxK	747.56	Joback Method
cpg	680.93	J/molxK	782.34	Joback Method
cpg	696.27	J/molxK	817.13	Joback Method
cpg	710.65	J/molxK	851.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009268&Units=SI
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

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
mccvol:	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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