

Aniline, 2-tert-butyl-n-sec-butyl-

Inchi:	InChI=1S/C14H23N/c1-6-11(2)15-13-10-8-7-9-12(13)14(3,4)5/h7-11,15H,6H2,1-5H3
InchiKey:	WBRFKMQTYCMFKI-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCC(C)Nc1ccccc1C(C)(C)C
Mol. weight [g/mol]:	205.34

Physical Properties

Property code	Value	Unit	Source
gf	259.57	kJ/mol	Joback Method
hf	-67.79	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	54.45	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.194		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	597.88	K	Joback Method
tc	809.14	K	Joback Method
tf	326.56	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.25	J/molxK	597.88	Joback Method
cpg	521.07	J/molxK	633.09	Joback Method
cpg	538.71	J/molxK	668.30	Joback Method
cpg	555.25	J/molxK	703.51	Joback Method
cpg	570.73	J/molxK	738.72	Joback Method
cpg	585.22	J/molxK	773.93	Joback Method
cpg	598.79	J/molxK	809.14	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=B6009272&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
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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