

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

Inchi:	InChI=1S/C13H21N/c1-6-14-12-8-7-11(9-10(12)2)13(3,4)5/h7-9,14H,6H2,1-5H3
InchiKey:	CMMYBXRNVGTZMI-UHFFFAOYSA-N
Formula:	C13H21N
SMILES:	CCNc1ccc(C(C)(C)C)cc1C
Mol. weight [g/mol]:	191.31

Physical Properties

Property code	Value	Unit	Source
gf	243.96	kJ/mol	Joback Method
hf	-53.34	kJ/mol	Joback Method
hfus	20.37	kJ/mol	Joback Method
hvap	53.27	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.724		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
tb	580.42	K	Joback Method
tc	791.78	K	Joback Method
tf	342.81	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.14	J/molxK	580.42	Joback Method
cpg	468.81	J/molxK	615.65	Joback Method
cpg	485.41	J/molxK	650.87	Joback Method
cpg	501.00	J/molxK	686.10	Joback Method
cpg	515.63	J/molxK	721.33	Joback Method
cpg	529.35	J/molxK	756.56	Joback Method
cpg	542.23	J/molxK	791.78	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=B6009274&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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