Aniline, n-allyl-o-tert-butyl-

Inchi: InChI=1S/C13H19N/c1-5-10-14-12-9-7-6-8-11(12)13(2,3)4/h5-9,14H,1,10H2,2-4H3
InchiKey: JTNWLMYDECZVFY-UHFFFAOYSA-N
Formula: C13H19N
SMILES: C=CCNc1ccccc1C(C)(C)C
Mol. weight [g/mol]: 189.30
CAS: 193338-72-6

Physical Properties

Property code	Value	Unit	Source
gf	341.43	kJ/mol	Joback Method
hf	83.56	kJ/mol	Joback Method
hfus	19.48	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.582		Crippen Method
mcvol	175.950	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	572.12	K	Joback Method
tc	786.85	K	Joback Method
tf	328.53	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.59	J/mol×K	572.12	Joback Method
cpg	447.98	J/mol×K	607.91	Joback Method
cpg	464.23	J/mol×K	643.70	Joback Method
cpg	479.41	J/mol×K	679.48	Joback Method
cpg	493.58	J/mol×K	715.27	Joback Method
cpg	506.80	J/mol×K	751.06	Joback Method
cpg	519.15	J/mol×K	786.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C193338726&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume