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

Inchi: InChI=1S/C11H17N/c1-9-5-7-10(8-6-9)12-11(2,3)4/h5-8,12H,1-4H3
InchiKey: XVOOKSRPDMBTAI-UHFFFAOYSA-N
Formula: C11H17N
SMILES: Cc1ccc(NC(C)(C)C)cc1
Mol. weight [g/mol]: 163.26
CAS: 10219-31-5

Physical Properties

Property code	Value	Unit	Source
gf	236.75	kJ/mol	Joback Method
hf	-0.59	kJ/mol	Joback Method
hfus	15.58	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.205		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	529.68	K	Joback Method
tc	747.19	K	Joback Method
tf	307.75	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.99	J/mol×K	529.68	Joback Method
cpg	370.79	J/mol×K	565.93	Joback Method
cpg	386.49	J/mol×K	602.18	Joback Method
cpg	401.16	J/mol×K	638.44	Joback Method
cpg	414.86	J/mol×K	674.69	Joback Method
cpg	427.64	J/mol×K	710.94	Joback Method
cpg	439.56	J/mol×K	747.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10219315&Units=SI
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

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