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

Other names: 4-tert-butyl-o-toluidine
Inchi: InChI=1S/C11H17N/c1-8-7-9(11(2,3)4)5-6-10(8)12/h5-7H,12H2,1-4H3
InchiKey: ZPWRNXCIWFCXOL-UHFFFAOYSA-N
Formula: C11H17N
SMILES: Cc1cc(C(C)(C)C)ccc1N
Mol. weight [g/mol]: 163.26
CAS: 2909-82-2

Physical Properties

Property code	Value	Unit	Source
gf	204.18	kJ/mol	Joback Method
hf	-31.74	kJ/mol	Joback Method
hfus	15.29	kJ/mol	Joback Method
hvap	53.03	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.875		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	557.02	K	Joback Method
tc	785.11	K	Joback Method
tf	350.87	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.85	J/mol×K	557.02	Joback Method
cpg	382.00	J/mol×K	595.03	Joback Method
cpg	397.09	J/mol×K	633.05	Joback Method
cpg	411.16	J/mol×K	671.06	Joback Method
cpg	424.29	J/mol×K	709.08	Joback Method
cpg	436.54	J/mol×K	747.09	Joback Method
cpg	447.95	J/mol×K	785.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2909822&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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume