

Aniline, m-tert-butyl-

Other names:	Aniline, 3-tert-butyl 3-tert-butylaniline
Inchi:	InChI=1S/C10H15N/c1-10(2,3)8-5-4-6-9(11)7-8/h4-7H,11H2,1-3H3
InchiKey:	DPKTVUKEPNBABS-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(C)(C)c1cccc(N)c1
Mol. weight [g/mol]:	149.23
CAS:	5369-19-7

Physical Properties

Property code	Value	Unit	Source
gf	205.39	kJ/mol	Joback Method
hf	0.37	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	50.14	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.566		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	529.16	K	Joback Method
tc	760.46	K	Joback Method
tf	327.08	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.50	J/mol×K	529.16	Joback Method
cpg	335.25	J/mol×K	567.71	Joback Method
cpg	349.89	J/mol×K	606.26	Joback Method
cpg	363.48	J/mol×K	644.81	Joback Method
cpg	376.10	J/mol×K	683.36	Joback Method
cpg	387.79	J/mol×K	721.91	Joback Method
cpg	398.65	J/mol×K	760.46	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=C5369197&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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