Benzoic acid, 3-amino-, tert.-butyl ester

Inchi: InChI=1S/C11H15NO2/c1-11(2,3)14-10(13)8-5-4-6-9(12)7-8/h4-7H,12H2,1-3H3
InchiKey: YGIRNXMYJLWFLH-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CC(C)(C)OC(=O)c1cccc(N)c1
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
gf	-20.11	kJ/mol	Joback Method
hf	-265.07	kJ/mol	Joback Method
hfus	18.47	kJ/mol	Joback Method
hvap	61.52	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.224		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1620.00		NIST Webbook
tb	628.33	K	Joback Method
tc	859.60	K	Joback Method
tf	410.51	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.98	J/mol×K	628.33	Joback Method
cpg	423.38	J/mol×K	666.87	Joback Method
cpg	436.77	J/mol×K	705.42	Joback Method
cpg	449.17	J/mol×K	743.96	Joback Method
cpg	460.64	J/mol×K	782.51	Joback Method
cpg	471.23	J/mol×K	821.05	Joback Method
cpg	480.99	J/mol×K	859.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375447&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume