tert-Butyl carbanilate

Other names:	Carbamic acid, phenyl-, 1,1-dimethylethyl ester
	Carbanilic acid, tert-butyl ester
	tert-Butyl phenylcarbamate
	tert-Butyl phenylurethane
	tert-Butyl N-phenylcarbamate
	tert-Butyl N-phenylurethane
	t-Butyl carbanilate
	N-Phenyl-O-tert-butylurethane
	Carbamic acid, phenyl, tert-butyl ester
	Carbamic acid, phenyl, tert.-butyl ester
	tert.-Butyl N-phenyl carbamate
Inchi:	InChI=1S/C11H15NO2/c1-11(2,3)14-10(13)12-9-7-5-4-6-8-9/h4-8H,1-3H3,(H,12,13)
InchiKey:	KZZHPWMVEVZEFG-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CC(C)(C)OC(=O)Nc1ccccc1
Mol. weight [g/mol]:	193.24
CAS:	3422-01-3

Physical Properties

Property code	Value	Unit	Source
gf	12.46	kJ/mol	Joback Method
hf	-233.92	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	56.65	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.034		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1465.00		NIST Webbook
ripol	1953.00		NIST Webbook
tb	600.99	K	Joback Method
tc	822.79	K	Joback Method
tf	367.39	K	Joback Method

vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.67	J/mol×K	600.99	Joback Method
cpg	414.69	J/mol×K	637.96	Joback Method
cpg	428.67	J/mol×K	674.92	Joback Method
cpg	441.65	J/mol×K	711.89	Joback Method
cpg	453.68	J/mol×K	748.86	Joback Method
cpg	464.81	J/mol×K	785.82	Joback Method
cpg	475.10	J/mol×K	822.79	Joback Method

Sources

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=C3422013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume