Benzoic acid, 3-(tert.-butyl)amino-, methyl ester

Inchi: InChI=1S/C12H17NO2/c1-12(2,3)13-10-7-5-6-9(8-10)11(14)15-4/h5-8,13H,1-4H3
InchiKey: IAJKNZYHCJHENC-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: COC(=O)c1cccc(NC(C)(C)C)c1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	11.25	kJ/mol	Joback Method
hf	-266.03	kJ/mol	Joback Method
hfus	20.96	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.684		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	628.85	K	Joback Method
tc	847.63	K	Joback Method
tf	391.18	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.58	J/mol×K	628.85	Joback Method
cpg	463.92	J/mol×K	665.31	Joback Method
cpg	478.24	J/mol×K	701.78	Joback Method
cpg	491.59	J/mol×K	738.24	Joback Method
cpg	504.00	J/mol×K	774.70	Joback Method
cpg	515.53	J/mol×K	811.16	Joback Method
cpg	526.22	J/mol×K	847.63	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=U375337&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume