Carbanilic acid, n-tert-butyl-, ethyl ester

Inchi: InChI=1S/C13H19NO2/c1-5-16-12(15)14(13(2,3)4)11-9-7-6-8-10-11/h6-10H,5H2,1-4H3
InchiKey: QXIJEOZQDPTADP-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCOC(=O)N(c1ccccc1)C(C)(C)C
Mol. weight [g/mol]: 221.30
CAS: 62603-73-0

Physical Properties

Property code	Value	Unit	Source
gf	50.69	kJ/mol	Joback Method
hf	-261.14	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.448		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
tb	609.02	K	Joback Method
tc	820.78	K	Joback Method
tf	369.74	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.86	J/mol×K	609.02	Joback Method
cpg	500.86	J/mol×K	644.31	Joback Method
cpg	516.73	J/mol×K	679.61	Joback Method
cpg	531.52	J/mol×K	714.90	Joback Method
cpg	545.29	J/mol×K	750.19	Joback Method
cpg	558.10	J/mol×K	785.48	Joback Method
cpg	570.00	J/mol×K	820.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62603730&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

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