Carbanilic acid, 2,4-di-tert-butyl-, ethyl ester

Inchi: InChI=1S/C17H27NO2/c1-8-20-15(19)18-14-10-9-12(16(2,3)4)11-13(14)17(5,6)7/h9-11H
InchiKey: FUOWRPLHFFSUJD-UHFFFAOYSA-N
Formula: C17H27NO2
SMILES: CCOC(=O)Nc1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
gf	46.56	kJ/mol	Joback Method
hf	-389.45	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.850		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
tb	745.00	K	Joback Method
tc	958.91	K	Joback Method
tf	462.47	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.48	J/mol×K	745.00	Joback Method
cpg	734.90	J/mol×K	780.65	Joback Method
cpg	751.16	J/mol×K	816.30	Joback Method
cpg	766.32	J/mol×K	851.95	Joback Method
cpg	780.46	J/mol×K	887.60	Joback Method
cpg	793.64	J/mol×K	923.26	Joback Method
cpg	805.94	J/mol×K	958.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009308&Units=SI

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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