Acetanilide, 2,4-di-tert-butyl-n-methyl-

Inchi: InChI=1S/C17H27NO/c1-12(19)18(8)15-10-9-13(16(2,3)4)11-14(15)17(5,6)7/h9-11H,1-8
InchiKey: AYGAAGMCZHPNQB-UHFFFAOYSA-N
Formula: C17H27NO
SMILES: CC(=O)N(C)c1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]: 261.40

Physical Properties

Property code	Value	Unit	Source
gf	172.95	kJ/mol	Joback Method
hf	-243.17	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.264		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
tb	684.85	K	Joback Method
tc	898.64	K	Joback Method
tf	420.05	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.40	J/mol×K	684.85	Joback Method
cpg	689.43	J/mol×K	720.48	Joback Method
cpg	707.19	J/mol×K	756.11	Joback Method
cpg	723.77	J/mol×K	791.74	Joback Method
cpg	739.25	J/mol×K	827.38	Joback Method
cpg	753.73	J/mol×K	863.01	Joback Method
cpg	767.30	J/mol×K	898.64	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=B6009287&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume