Acetanilide, n,4-ditertiary butyl-

Inchi: InChI=1S/C16H25NO/c1-12(18)17(16(5,6)7)14-10-8-13(9-11-14)15(2,3)4/h8-11H,1-7H3
InchiKey: RNPTWGQJUXZCLZ-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CC(=O)N(c1ccc(C(C)(C)C)cc1)C(C)(C)C
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	174.16	kJ/mol	Joback Method
hf	-211.06	kJ/mol	Joback Method
hfus	20.64	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.136		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
tb	656.99	K	Joback Method
tc	873.38	K	Joback Method
tf	396.26	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.07	J/mol×K	656.99	Joback Method
cpg	635.15	J/mol×K	693.05	Joback Method
cpg	652.88	J/mol×K	729.12	Joback Method
cpg	669.38	J/mol×K	765.18	Joback Method
cpg	684.72	J/mol×K	801.25	Joback Method
cpg	699.02	J/mol×K	837.31	Joback Method
cpg	712.38	J/mol×K	873.38	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=B6009285&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

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