

Acetanilide, 2,6-diethyl-4-tert-butyl-

Inchi: InChI=1S/C16H25NO/c1-7-12-9-14(16(4,5)6)10-13(8-2)15(12)17-11(3)18/h9-10H,7-8H2,
InchiKey: OSSFCCXGYSEKLZ-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCc1cc(C(C)(C)C)cc(CC)c1N=C(C)O
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
hf	-260.00	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.717		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
tb	772.61	K	Joback Method
tc	979.95	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009293&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation 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

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