

Acetanilide, 2,6-di-isopropyl-4-tert-butyl-

Inchi:	InChI=1S/C18H29NO/c1-11(2)15-9-14(18(6,7)8)10-16(12(3)4)17(15)19-13(5)20/h9-12H,
InchiKey:	BQEQSRVMHCNBTU-UHFFFAOYSA-N
Formula:	C18H29NO
SMILES:	CC(O)=Nc1c(C(C)C)cc(C(C)(C)C)cc1C(C)C
Mol. weight [g/mol]:	275.43

Physical Properties

Property code	Value	Unit	Source
hf	-311.84	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.839		Crippen Method
mccvol	252.270	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
tb	817.49	K	Joback Method
tc	1027.39	K	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=B6009295&Units=SI

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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