

Acetanilide, 2,6-diisopropyl-

Inchi: InChI=1S/C14H21NO/c1-9(2)12-7-6-8-13(10(3)4)14(12)15-11(5)16/h6-10H,1-5H3,(H,15,
InchiKey: FBMIRBWQIPKRAB-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CC(O)=Nc1c(C(C)C)cccc1C(C)C
Mol. weight [g/mol]: 219.32
CAS: 16637-13-1

Physical Properties

Property code	Value	Unit	Source
hf	-209.06	kJ/mol	Joback Method
hvap	69.66	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.541		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
tb	724.22	K	Joback Method
tc	932.50	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=C16637131&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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