2,6-diethylacetanilide

Inchi: InChI=1S/C12H17NO/c1-4-10-7-6-8-11(5-2)12(10)13-9(3)14/h6-8H,4-5H2,1-3H3,(H,13,1
InchiKey: SNPZDXACCGIJNK-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCc1cccc(CC)c1N=C(C)O
Mol. weight [g/mol]: 191.27
CAS: 16665-89-7

Physical Properties

Property code	Value	Unit	Source
hf	-157.22	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.419		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	679.34	K	Joback Method
tc	885.93	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16665897&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature