Benzamide, 3-methyl-N-(2-ethylhexyl)-

Inchi: InChI=1S/C16H25NO/c1-4-6-9-14(5-2)12-17-16(18)15-10-7-8-13(3)11-15/h7-8,10-11,14H
InchiKey: PVGAZWSAFDFZLF-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCC(CC)CN=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
hf	-233.59	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.516		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
tb	765.44	K	Joback Method
tc	966.12	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407416&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

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