3-Methyl-N-naphthalen-1-yl-benzamide

Other names: Benzamide, N-(1-naphthyl)-3-methyl-
Inchi: InChI=1S/C18H15NO/c1-13-6-4-9-15(12-13)18(20)19-17-11-5-8-14-7-2-3-10-16(14)17/h
InchiKey: YORPYFLFOLLPND-UHFFFAOYSA-N
Formula: C18H15NO
SMILES: Cc1cccc(C(O)=Nc2cccc3ccccc23)c1
Mol. weight [g/mol]: 261.32
CAS: 96963-49-4

Physical Properties

Property code	Value	Unit	Source
hf	146.54	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.785		Crippen Method
mcvol	209.050	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2603.00		NIST Webbook
rinpol	2603.00		NIST Webbook
tb	862.28	K	Joback Method
tc	1107.44	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96963494&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

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