

N,N-Dimethyl-N'-heptyl-p-methoxybenzamide

Inchi: InChI=1S/C17H28N2O/c1-5-6-7-8-9-14-18-17(19(2)3)15-10-12-16(20-4)13-11-15/h10-13
InchiKey: QFHFTBAGZBCXJE-ISLYRVAYSA-N
Formula: C17H28N2O
SMILES: CCCCCCN=C(c1ccc(OC)cc1)N(C)C
Mol. weight [g/mol]: 276.42

Physical Properties

Property code	Value	Unit	Source
hf	-161.41	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.974		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2012.00		NIST Webbook
tb	731.44	K	Joback Method
tc	932.65	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R159232&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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