N,N-Dimethyl-N'-(3-nitrophenyl)-p-methoxybenzar

Inchi: InChI=1S/C16H17N3O3/c1-18(2)16(12-7-9-15(22-3)10-8-12)17-13-5-4-6-14(11-13)19(20
InchiKey: LPYKLRFCAWMZKP-UHFFFAOYSA-N
Formula: C16H17N3O3
SMILES: COc1ccc(C(=Nc2cccc([N+](=O)[O-])c2)N(C)C)cc1
Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
hf	73.53	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.243		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	892.06	K	Joback Method
tc	1150.04	K	Joback Method

Sources

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=R158799&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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