

N,N-Dimethyl-N'-(3-ethoxyphenyl)-propionamide

Inchi: InChI=1S/C13H20N2O/c1-5-13(15(3)4)14-11-8-7-9-12(10-11)16-6-2/h7-10H,5-6H2,1-4H3
InchiKey: QIBWMUWWJGRKSI-UHFFFAOYSA-N
Formula: C13H20N2O
SMILES: CCOc1cccc(N=C(CC)N(C)C)c1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
hf	-78.85	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	3.087		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1793.00		NIST Webbook
tb	639.92	K	Joback Method
tc	851.78	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R161903&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

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