

N-(3-Ethoxyphenyl)-N'-(3-chlorophenyl)formamidi

Inchi: InChI=1S/C15H15BrN2O/c1-2-19-15-8-4-7-14(10-15)18-11-17-13-6-3-5-12(16)9-13/h3-1
InchiKey: ZZIDLONYOBSYMW-UHFFFAOYSA-N
Formula: C15H15BrN2O
SMILES: CCOc1cccc(NC=Nc2cccc(Br)c2)c1
Mol. weight [g/mol]: 319.20

Physical Properties

Property code	Value	Unit	Source
hf	126.99	kJ/mol	Joback Method
hvap	73.46	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.620		Crippen Method
mcvol	213.720	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2509.00		NIST Webbook
tb	821.35	K	Joback Method
tc	1074.36	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R161527&Units=SI>
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

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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