Butanamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C11H15NO/c1-3-5-11(13)12-10-7-4-6-9(2)8-10/h4,6-8H,3,5H2,1-2H3,(H,12,13)
InchiKey: HHJVHZGGWADBKL-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCCC(O)=Nc1cccc(C)c1
Mol. weight [g/mol]: 177.24
CAS: 69833-26-7

Physical Properties

Property code	Value	Unit	Source
hf	-125.11	kJ/mol	Joback Method
hvap	63.09	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.383		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	651.48	K	Joback Method
tc	860.19	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69833267&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