

Propanamide, N-(3-methylphenyl)-2-bromo-

Inchi:	InChI=1S/C10H12BrNO/c1-7-4-3-5-9(6-7)12-10(13)8(2)11/h3-6,8H,1-2H3,(H,12,13)
InchiKey:	JWZPPAQMKDCYJG-UHFFFAOYSA-N
Formula:	C10H12BrNO
SMILES:	<chem>Cc1cccc(N=C(O)C(C)Br)c1</chem>
Mol. weight [g/mol]:	242.11

Physical Properties

Property code	Value	Unit	Source
hf	-83.42	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.366		Crippen Method
mcpvol	157.050	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
tb	694.32	K	Joback Method
tc	921.64	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307475&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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