Benzamide, 3-bromo-N-methyl-

Inchi: InChI=1S/C8H8BrNO/c1-10-8(11)6-3-2-4-7(9)5-6/h2-5H,1H3,(H,10,11)
InchiKey: YBNPCJSZMYHDDR-UHFFFAOYSA-N
Formula: C8H8BrNO
SMILES: CN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 214.06

Physical Properties

Property code	Value	Unit	Source
hf	-36.86	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.384		Crippen Method
mcvol	128.870	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1722.00		NIST Webbook
rinpol	1722.00		NIST Webbook
tb	649.00	K	Joback Method
tc	880.53	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407200&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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