Benzamide, 2-bromo-N-propyl-

Inchi: InChI=1S/C10H12BrNO/c1-2-7-12-10(13)8-5-3-4-6-9(8)11/h3-6H,2,7H2,1H3,(H,12,13)
InchiKey: XNIZYPMLUVRLJS-UHFFFAOYSA-N
Formula: C10H12BrNO
SMILES: CCCN=C(O)c1ccccc1Br
Mol. weight [g/mol]: 242.11

Physical Properties

Property code	Value	Unit	Source
hf	-78.14	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.164		Crippen Method
mcvol	157.050	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	694.76	K	Joback Method
tc	917.81	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407112&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