Benzamide, 3-bromo-N-undecyl-

Inchi: InChI=1S/C18H28BrNO/c1-2-3-4-5-6-7-8-9-10-14-20-18(21)16-12-11-13-17(19)15-16/h1
InchiKey: KEEMLTCAXXBORZ-UHFFFAOYSA-N
Formula: C18H28BrNO
SMILES: CCCCCCCCCCCN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 354.32

Physical Properties

Property code	Value	Unit	Source
hf	-243.26	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.284		Crippen Method
mcvol	269.770	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	877.80	K	Joback Method
tc	1086.27	K	Joback Method

Sources

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=U407214&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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