

Benzamide, 2-bromo-N-dodecyl-

Inchi: InChI=1S/C19H30BrNO/c1-2-3-4-5-6-7-8-9-10-13-16-21-19(22)17-14-11-12-15-18(17)20
InchiKey: OVSGJPLVQMQLDL-UHFFFAOYSA-N
Formula: C19H30BrNO
SMILES: CCCCCCCCCCN=C(O)c1cccc1Br
Mol. weight [g/mol]: 368.35

Physical Properties

Property code	Value	Unit	Source
hf	-263.90	kJ/mol	Joback Method
hvap	87.33	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.675		Crippen Method
mcvol	283.860	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	900.68	K	Joback Method
tc	1110.23	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407123&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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