Benzamide, 3-bromo-N-tetradecyl-

Inchi: InChI=1S/C21H34BrNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-23-21(24)19-15-14-16-20(22
InchiKey: NTXFVQBNSHPVDW-UHFFFAOYSA-N
Formula: C21H34BrNO
SMILES: CCCCCCCCCCCCCCN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 396.40

Physical Properties

Property code	Value	Unit	Source
hf	-305.18	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	7.455		Crippen Method
mcvol	312.040	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	3020.00		NIST Webbook
rinpol	3020.00		NIST Webbook
tb	946.44	K	Joback Method
tc	1160.62	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407216&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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