Benzamide, 3-bromo-N-octadecyl-

Inchi: InChI=1S/C25H42BrNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-27-25(28)23-19
InchiKey: UAEFEKPSYMWCKE-UHFFFAOYSA-N
Formula: C25H42BrNO
SMILES: CCCCCCCCCCCCCCCCCCN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 452.51

Physical Properties

Property code	Value	Unit	Source
hf	-387.74	kJ/mol	Joback Method
hvap	100.69	kJ/mol	Joback Method
log10ws	-9.64		Crippen Method
logp	9.015		Crippen Method
mcvol	368.400	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	3475.00		NIST Webbook
rinpol	3475.00		NIST Webbook
tb	1037.96	K	Joback Method
tc	1273.11	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=U407218&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