

Benzamide, 3-bromo-N-hexadecyl-

Inchi: InChI=1S/C23H38BrNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-25-23(26)21-17-16-18
InchiKey: RHFSUPAWCIKFQQ-UHFFFAOYSA-N
Formula: C23H38BrNO
SMILES: CCCCCCCCCCCCCCN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 424.46

Physical Properties

Property code	Value	Unit	Source
hf	-346.46	kJ/mol	Joback Method
hvap	96.24	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	8.235		Crippen Method
mcvol	340.220	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	3225.00		NIST Webbook
rinpol	3225.00		NIST Webbook
tb	992.20	K	Joback Method
tc	1214.73	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407217&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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