Benzamide, 3-bromo-N-(hept-2-yl)-

Inchi: InChI=1S/C14H20BrNO/c1-3-4-5-7-11(2)16-14(17)12-8-6-9-13(15)10-12/h6,8-11H,3-5,7
InchiKey: HUXXLRPTXAKIIZ-UHFFFAOYSA-N
Formula: C14H20BrNO
SMILES: CCCCCC(C)N=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 298.22

Physical Properties

Property code	Value	Unit	Source
hf	-165.98	kJ/mol	Joback Method
hvap	75.82	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.723		Crippen Method
mcvol	213.410	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	785.84	K	Joback Method
tc	1000.15	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407207&Units=SI

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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