

# Hexanamide, N,N-dioctyl-6-bromo-

<b>Inchi:</b>	InChI=1S/C22H44BrNO/c1-3-5-7-9-11-16-20-24(21-17-12-10-8-6-4-2)22(25)18-14-13-15
<b>InchiKey:</b>	WFGNURHFUXIZTC-UHFFFAOYSA-N
<b>Formula:</b>	C22H44BrNO
<b>SMILES:</b>	CCCCCCCCN(CCCCCCCC)C(=O)CCCCBr
<b>Mol. weight [g/mol]:</b>	418.50

## Physical Properties

Property code	Value	Unit	Source
gf	130.54	kJ/mol	Joback Method
hf	-516.13	kJ/mol	Joback Method
hfus	62.64	kJ/mol	Joback Method
hvap	79.79	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.491		Crippen Method
mcvol	349.890	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	835.23	K	Joback Method
tc	1023.47	K	Joback Method
tf	479.90	K	Joback Method
vc	1.353	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.39	J/molxK	835.23	Joback Method
cpg	1117.17	J/molxK	866.60	Joback Method
cpg	1135.92	J/molxK	897.98	Joback Method
cpg	1153.69	J/molxK	929.35	Joback Method
cpg	1170.55	J/molxK	960.72	Joback Method
cpg	1186.55	J/molxK	992.10	Joback Method
cpg	1201.75	J/molxK	1023.47	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308652&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308652&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/95-910-6/Hexanamide-N-N-dioctyl-6-bromo.pdf>

Generated by Cheméo on 2024-04-30 15:19:58.756538876 +0000 UTC m=+16779647.677116191.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.