

# «beta»-Alanine, N-(3-bromobenzoyl)-, octyl ester

Inchi:	InChI=1S/C18H26BrNO3/c1-2-3-4-5-6-7-13-23-17(21)11-12-20-18(22)15-9-8-10-16(19)1
InchiKey:	DGCBFNDBOHLFMZ-UHFFFAOYSA-N
Formula:	C18H26BrNO3
SMILES:	CCCCCCCCOC(=O)CCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	384.31

## Physical Properties

Property code	Value	Unit	Source
gf	-55.67	kJ/mol	Joback Method
hf	-467.37	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.473		Crippen Method
mcvol	277.210	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinsol	2795.00		NIST Webbook
tb	889.39	K	Joback Method
tc	1102.72	K	Joback Method
tf	566.11	K	Joback Method
vc	1.062	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.43	J/mol×K	889.39	Joback Method
cpg	843.18	J/mol×K	924.94	Joback Method
cpg	855.90	J/mol×K	960.50	Joback Method
cpg	867.65	J/mol×K	996.05	Joback Method
cpg	878.47	J/mol×K	1031.61	Joback Method
cpg	888.41	J/mol×K	1067.16	Joback Method
cpg	897.52	J/mol×K	1102.72	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=U321645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321645&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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/30-559-8/beta-Alanine-N-3-bromobenzoyl-octyl-ester.pdf>

Generated by Cheméo on 2024-04-23 21:21:29.399170579 +0000 UTC m=+16196538.319747894.

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