

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

Inchi:	InChI=1S/C19H28BrNO3/c1-2-3-4-5-6-7-8-14-24-18(22)12-13-21-19(23)16-10-9-11-17(2
InchiKey:	QYRGPDVIPUGGPI-UHFFFAOYSA-N
Formula:	C19H28BrNO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	398.33

Physical Properties

Property code	Value	Unit	Source
gf	-47.25	kJ/mol	Joback Method
hf	-488.01	kJ/mol	Joback Method
hfus	53.39	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.863		Crippen Method
mcvol	291.300	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinsol	2930.00		NIST Webbook
tb	912.27	K	Joback Method
tc	1126.24	K	Joback Method
tf	577.38	K	Joback Method
vc	1.119	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.92	J/mol×K	912.27	Joback Method
cpg	901.92	J/mol×K	947.93	Joback Method
cpg	914.87	J/mol×K	983.59	Joback Method
cpg	926.82	J/mol×K	1019.25	Joback Method
cpg	937.82	J/mol×K	1054.91	Joback Method
cpg	947.93	J/mol×K	1090.58	Joback Method
cpg	957.18	J/mol×K	1126.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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