.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]: 398.34

Physical Properties

Property code	Value	Unit	Source
hf	-632.05	kJ/mol	Cheméo Relay (1.0)
hfus	53.39	kJ/mol	Joback Method
hvap	114.32	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-6.03		Cheméo Relay (1.0)
logp	4.863		Crippen Method
mcvol	291.300	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	2930.00		NIST Webbook
tb	667.79	K	Cheméo Relay (1.0)
tf	320.05	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321646&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point