«beta»-Alanine, N-(2-bromobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C22H34BrNO3/c1-2-3-4-5-6-7-8-9-10-13-18-27-21(25)16-17-24-22(26)19-14-1

InchiKey: NBKYWDHFSGYNII-UHFFFAOYSA-N

Formula: C22H34BrNO3

SMILES: CCCCCCCCCCCCOC(=O)CCNC(=O)c1ccccc1Br

Mol. weight [g/mol]: 440.41

Physical Properties

Property code	Value	Unit	Source
gf	-21.99	kJ/mol	Joback Method
hf	-549.93	kJ/mol	Joback Method
hfus	61.16	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.033		Crippen Method
mcvol	333.570	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	3487.00		NIST Webbook
rinpol	3487.00		NIST Webbook
tb	980.91	K	Joback Method
tc	1201.88	K	Joback Method
tf	611.19	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.43	J/mol×K	980.91	Joback Method
cpg	1082.25	J/mol×K	1017.74	Joback Method
cpg	1095.92	J/mol×K	1054.57	Joback Method
cpg	1108.49	J/mol×K	1091.40	Joback Method
cpg	1120.03	J/mol×K	1128.22	Joback Method
cpg	1130.61	J/mol×K	1165.05	Joback Method
cpg	1140.29	J/mol×K	1201.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321736&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume