

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

Inchi:	InChI=1S/C22H34BrNO3/c1-2-3-4-5-6-7-8-9-10-11-17-27-21(25)15-16-24-22(26)19-13-1
InchiKey:	QCPLRMLWHRZURK-UHFFFAOYSA-N
Formula:	C22H34BrNO3
SMILES:	CCCCCCCCCCCCOC(=O)CCNC(=O)c1cccc(Br)c1
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
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/molxK	980.91	Joback Method
cpg	1082.25	J/molxK	1017.74	Joback Method
cpg	1095.92	J/molxK	1054.57	Joback Method
cpg	1108.49	J/molxK	1091.40	Joback Method
cpg	1120.03	J/molxK	1128.22	Joback Method
cpg	1130.61	J/molxK	1165.05	Joback Method
cpg	1140.29	J/molxK	1201.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321649&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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