

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

Inchi:	InChI=1S/C21H32BrNO3/c1-2-3-4-5-6-7-8-9-10-16-26-20(24)14-15-23-21(25)18-12-11-1
InchiKey:	LGUUMYATIYASBJ-UHFFFAOYSA-N
Formula:	C21H32BrNO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	426.39

Physical Properties

Property code	Value	Unit	Source
gf	-30.41	kJ/mol	Joback Method
hf	-529.29	kJ/mol	Joback Method
hfus	58.57	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	5.643		Crippen Method
mvol	319.480	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	3286.00		NIST Webbook
rinpol	3286.00		NIST Webbook
tb	958.03	K	Joback Method
tc	1175.76	K	Joback Method
tf	599.92	K	Joback Method
vc	1.230	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.97	J/mol×K	958.03	Joback Method
cpg	1021.50	J/mol×K	994.32	Joback Method
cpg	1034.91	J/mol×K	1030.61	Joback Method
cpg	1047.27	J/mol×K	1066.90	Joback Method
cpg	1058.62	J/mol×K	1103.18	Joback Method
cpg	1069.04	J/mol×K	1139.47	Joback Method
cpg	1078.59	J/mol×K	1175.76	Joback Method

Sources

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=U321648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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