«beta»-Alanine, N-(4-chlorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C21H32ClNO3/c1-2-3-4-5-6-7-8-9-10-17-26-20(24)15-16-23-21(25)18-11-13-1

InchiKey: IRWQMPMLJWACMD-UHFFFAOYSA-N

Formula: C21H32ClNO3

SMILES: CCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 381.94

Physical Properties

Property code	Value	Unit	Source
gf	-56.66	kJ/mol	Joback Method
hf	-571.36	kJ/mol	Joback Method
hfus	57.48	kJ/mol	Joback Method
hvap	92.00	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.534		Crippen Method
mcvol	314.220	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	3138.00		NIST Webbook
rinpol	3138.00		NIST Webbook
tb	929.30	K	Joback Method
tc	1140.86	K	Joback Method
tf	570.04	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.05	J/mol×K	929.30	Joback Method
cpg	1009.00	J/mol×K	964.56	Joback Method
cpg	1022.80	J/mol×K	999.82	Joback Method
cpg	1035.50	J/mol×K	1035.08	Joback Method
cpg	1047.13	J/mol×K	1070.34	Joback Method
cpg	1057.75	J/mol×K	1105.60	Joback Method
cpg	1067.41	J/mol×K	1140.86	Joback Method

Sources

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=U321725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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