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

Inchi: InChI=1S/C20H30ClNO3/c1-2-3-4-5-6-7-8-9-16-25-19(23)14-15-22-20(24)17-10-12-18(2

InchiKey: YCYJYQKVEYADGA-UHFFFAOYSA-N

Formula: C20H30ClNO3

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

Mol. weight [g/mol]: 367.91

Physical Properties

Property code	Value	Unit	Source
gf	-65.08	kJ/mol	Joback Method
hf	-550.72	kJ/mol	Joback Method
hfus	54.89	kJ/mol	Joback Method
hvap	89.77	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.144		Crippen Method
mcvol	300.130	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2967.00		NIST Webbook
tb	906.42	K	Joback Method
tc	1115.72	K	Joback Method
tf	558.77	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.33	J/mol×K	906.42	Joback Method
cpg	949.03	J/mol×K	941.30	Joback Method
cpg	962.62	J/mol×K	976.19	Joback Method
cpg	975.14	J/mol×K	1011.07	Joback Method
cpg	986.63	J/mol×K	1045.95	Joback Method
cpg	997.15	J/mol×K	1080.83	Joback Method
cpg	1006.72	J/mol×K	1115.72	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=U321724&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