Sarcosine, N-(2-chlorobenzoyl)-, pentyl ester

Inchi: InChI=1S/C15H20ClNO3/c1-3-4-7-10-20-14(18)11-17(2)15(19)12-8-5-6-9-13(12)16/h5-6
InchiKey: KELZJYIYVCWDRO-UHFFFAOYSA-N
Formula: C15H20ClNO3
SMILES: CCCCCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 297.78

Physical Properties

Property code	Value	Unit	Source
gf	-85.79	kJ/mol	Joback Method
hf	-433.46	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.145		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	754.29	K	Joback Method
tc	960.82	K	Joback Method
tf	482.23	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.22	J/mol×K	754.29	Joback Method
cpg	647.38	J/mol×K	788.71	Joback Method
cpg	660.57	J/mol×K	823.13	Joback Method
cpg	672.83	J/mol×K	857.55	Joback Method
cpg	684.20	J/mol×K	891.97	Joback Method
cpg	694.71	J/mol×K	926.40	Joback Method
cpg	704.40	J/mol×K	960.82	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=U321205&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