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

Inchi: InChI=1S/C12H14ClNO3/c1-3-17-11(15)8-14(2)12(16)9-6-4-5-7-10(9)13/h4-7H,3,8H2,1-2
InchiKey: RBBWFAMCKUUJGX-UHFFFAOYSA-N
Formula: C12H14ClNO3
SMILES: CCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 255.70

Physical Properties

Property code	Value	Unit	Source
gf	-111.05	kJ/mol	Joback Method
hf	-371.54	kJ/mol	Joback Method
hfus	32.09	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.975		Crippen Method
mcvol	187.410	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1928.00		NIST Webbook
tb	685.65	K	Joback Method
tc	900.24	K	Joback Method
tf	448.42	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.52	J/mol×K	685.65	Joback Method
cpg	487.43	J/mol×K	721.42	Joback Method
cpg	499.45	J/mol×K	757.18	Joback Method
cpg	510.61	J/mol×K	792.95	Joback Method
cpg	520.93	J/mol×K	828.71	Joback Method
cpg	530.44	J/mol×K	864.48	Joback Method
cpg	539.18	J/mol×K	900.24	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=U321202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume