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

Inchi: InChI=1S/C22H34ClNO3/c1-3-4-5-6-7-8-9-10-11-14-17-27-21(25)18-24(2)22(26)19-15-1
InchiKey: QNPJVNNCUBIYBF-UHFFFAOYSA-N
Formula: C22H34ClNO3
SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 395.96

Physical Properties

Property code	Value	Unit	Source
gf	-26.85	kJ/mol	Joback Method
hf	-577.94	kJ/mol	Joback Method
hfus	57.99	kJ/mol	Joback Method
hvap	89.83	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.876		Crippen Method
mcvol	328.310	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	3036.00		NIST Webbook
tb	914.45	K	Joback Method
tc	1122.44	K	Joback Method
tf	561.12	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.17	J/mol×K	914.45	Joback Method
cpg	1054.18	J/mol×K	949.11	Joback Method
cpg	1069.03	J/mol×K	983.78	Joback Method
cpg	1082.78	J/mol×K	1018.44	Joback Method
cpg	1095.49	J/mol×K	1053.11	Joback Method
cpg	1107.20	J/mol×K	1087.77	Joback Method
cpg	1117.98	J/mol×K	1122.44	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=U321211&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