Sarcosine, N-(4-chlorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C21H32ClNO3/c1-3-4-5-6-7-8-9-10-11-16-26-20(24)17-23(2)21(25)18-12-14-1
InchiKey: GJYSOEJLPGTJJA-UHFFFAOYSA-N
Formula: C21H32ClNO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 381.94

Physical Properties

Property code	Value	Unit	Source
gf	-35.27	kJ/mol	Joback Method
hf	-557.30	kJ/mol	Joback Method
hfus	55.40	kJ/mol	Joback Method
hvap	87.61	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.486		Crippen Method
mcvol	314.220	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	891.57	K	Joback Method
tc	1097.17	K	Joback Method
tf	549.85	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.96	J/mol×K	891.57	Joback Method
cpg	993.70	J/mol×K	925.84	Joback Method
cpg	1008.33	J/mol×K	960.10	Joback Method
cpg	1021.88	J/mol×K	994.37	Joback Method
cpg	1034.42	J/mol×K	1028.64	Joback Method
cpg	1046.00	J/mol×K	1062.91	Joback Method
cpg	1056.66	J/mol×K	1097.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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