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

Inchi: InChI=1S/C20H30ClNO3/c1-3-4-5-6-7-8-9-12-15-25-19(23)16-22(2)20(24)17-13-10-11-1
InchiKey: ZNCTXOPPEHUQQW-UHFFFAOYSA-N
Formula: C20H30ClNO3
SMILES: CCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 367.91

Physical Properties

Property code	Value	Unit	Source
gf	-43.69	kJ/mol	Joback Method
hf	-536.66	kJ/mol	Joback Method
hfus	52.81	kJ/mol	Joback Method
hvap	85.38	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.096		Crippen Method
mcvol	300.130	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	868.69	K	Joback Method
tc	1072.72	K	Joback Method
tf	538.58	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.44	J/mol×K	868.69	Joback Method
cpg	933.93	J/mol×K	902.70	Joback Method
cpg	948.33	J/mol×K	936.70	Joback Method
cpg	961.70	J/mol×K	970.71	Joback Method
cpg	974.08	J/mol×K	1004.71	Joback Method
cpg	985.51	J/mol×K	1038.72	Joback Method
cpg	996.06	J/mol×K	1072.72	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=U321210&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