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

Inchi: InChI=1S/C16H22ClNO3/c1-3-4-5-8-11-21-15(19)12-18(2)16(20)13-9-6-7-10-14(13)17/h
InchiKey: CCRNYVLCQLBOBV-UHFFFAOYSA-N
Formula: C16H22ClNO3
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 311.80

Physical Properties

Property code	Value	Unit	Source
gf	-77.37	kJ/mol	Joback Method
hf	-454.10	kJ/mol	Joback Method
hfus	42.45	kJ/mol	Joback Method
hvap	76.48	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.536		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2330.00		NIST Webbook
tb	777.17	K	Joback Method
tc	981.98	K	Joback Method
tf	493.50	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.39	J/mol×K	777.17	Joback Method
cpg	702.86	J/mol×K	811.31	Joback Method
cpg	716.34	J/mol×K	845.44	Joback Method
cpg	728.87	J/mol×K	879.58	Joback Method
cpg	740.49	J/mol×K	913.71	Joback Method
cpg	751.24	J/mol×K	947.85	Joback Method
cpg	761.15	J/mol×K	981.98	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=U321206&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