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

Inchi: InChI=1S/C17H24ClNO3/c1-3-4-5-6-9-12-22-16(20)13-19(2)17(21)14-10-7-8-11-15(14)1
InchiKey: DSQPSAANSXWBOD-UHFFFAOYSA-N
Formula: C17H24ClNO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 325.83

Physical Properties

Property code	Value	Unit	Source
gf	-68.95	kJ/mol	Joback Method
hf	-474.74	kJ/mol	Joback Method
hfus	45.04	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.926		Crippen Method
mcvol	257.860	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2436.00		NIST Webbook
tb	800.05	K	Joback Method
tc	1003.71	K	Joback Method
tf	504.77	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.57	J/mol×K	800.05	Joback Method
cpg	759.31	J/mol×K	833.99	Joback Method
cpg	773.05	J/mol×K	867.94	Joback Method
cpg	785.82	J/mol×K	901.88	Joback Method
cpg	797.66	J/mol×K	935.82	Joback Method
cpg	808.61	J/mol×K	969.77	Joback Method
cpg	818.71	J/mol×K	1003.71	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=U321207&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