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

Inchi: InChI=1S/C14H18ClNO3/c1-3-4-9-19-13(17)10-16(2)14(18)11-5-7-12(15)8-6-11/h5-8H,3
InchiKey: SRIOEDMSFBSNRU-UHFFFAOYSA-N
Formula: C14H18ClNO3
SMILES: CCCCOC(=O)CN(C)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 283.75

Physical Properties

Property code	Value	Unit	Source
gf	-94.21	kJ/mol	Joback Method
hf	-412.82	kJ/mol	Joback Method
hfus	37.27	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.755		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	731.41	K	Joback Method
tc	940.17	K	Joback Method
tf	470.96	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.14	J/mol×K	731.41	Joback Method
cpg	592.94	J/mol×K	766.20	Joback Method
cpg	605.80	J/mol×K	801.00	Joback Method
cpg	617.75	J/mol×K	835.79	Joback Method
cpg	628.82	J/mol×K	870.58	Joback Method
cpg	639.05	J/mol×K	905.37	Joback Method
cpg	648.47	J/mol×K	940.17	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321349&Units=SI

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