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

Inchi: InChI=1S/C16H22ClNO3/c1-12(2)5-4-10-21-15(19)11-18(3)16(20)13-6-8-14(17)9-7-13/h
InchiKey: QKNRAHQLPYVFFY-UHFFFAOYSA-N
Formula: C16H22ClNO3
SMILES: CC(C)CCCOC(=O)CN(C)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 311.80

Physical Properties

Property code	Value	Unit	Source
gf	-79.81	kJ/mol	Joback Method
hf	-459.38	kJ/mol	Joback Method
hfus	38.93	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.391		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	776.73	K	Joback Method
tc	984.39	K	Joback Method
tf	478.50	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.95	J/mol×K	776.73	Joback Method
cpg	703.62	J/mol×K	811.34	Joback Method
cpg	717.26	J/mol×K	845.95	Joback Method
cpg	729.92	J/mol×K	880.56	Joback Method
cpg	741.64	J/mol×K	915.17	Joback Method
cpg	752.45	J/mol×K	949.78	Joback Method
cpg	762.39	J/mol×K	984.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321351&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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