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

Inchi: InChI=1S/C13H16ClNO3/c1-3-8-18-12(16)9-15(2)13(17)10-6-4-5-7-11(10)14/h4-7H,3,8-9
InchiKey: MIFLCFDAVSUCKU-UHFFFAOYSA-N
Formula: C13H16ClNO3
SMILES: CCCOC(=O)CN(C)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 269.72

Physical Properties

Property code	Value	Unit	Source
gf	-102.63	kJ/mol	Joback Method
hf	-392.18	kJ/mol	Joback Method
hfus	34.68	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.365		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2029.00		NIST Webbook
tb	708.53	K	Joback Method
tc	919.99	K	Joback Method
tf	459.69	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.21	J/mol×K	708.53	Joback Method
cpg	539.60	J/mol×K	743.77	Joback Method
cpg	552.07	J/mol×K	779.02	Joback Method
cpg	563.66	J/mol×K	814.26	Joback Method
cpg	574.38	J/mol×K	849.50	Joback Method
cpg	584.29	J/mol×K	884.75	Joback Method
cpg	593.39	J/mol×K	919.99	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=U321203&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