l-Phenylalanine, N-(2-chlorobenzoyl)-, methyl ester

Inchi: InChI=1S/C17H16ClNO3/c1-22-17(21)15(11-12-7-3-2-4-8-12)19-16(20)13-9-5-6-10-14(1

InchiKey: SBBIHHYZJMQAMT-UHFFFAOYSA-N

Formula: C17H16ClNO3

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1ccccc1Cl

Mol. weight [g/mol]: 317.77

Physical Properties

Property code	Value	Unit	Source
gf	19.63	kJ/mol	Joback Method
hf	-257.55	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	84.98	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	2.854		Crippen Method
mcvol	234.100	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	864.02	K	Joback Method
tc	1103.34	K	Joback Method
tf	536.38	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.97	J/mol×K	864.02	Joback Method
cpg	674.10	J/mol×K	903.91	Joback Method
cpg	685.03	J/mol×K	943.79	Joback Method
cpg	694.83	J/mol×K	983.68	Joback Method
cpg	703.54	J/mol×K	1023.56	Joback Method
cpg	711.25	J/mol×K	1063.45	Joback Method
cpg	718.00	J/mol×K	1103.34	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=U299591&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