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

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

Physical Properties

Property code	Value	Unit	Source
gf	-128.90	kJ/mol	Joback Method
hf	-416.80	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.267		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1913.00		NIST Webbook
tb	745.38	K	Joback Method
tc	966.33	K	Joback Method
tf	449.88	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.01	J/mol×K	745.38	Joback Method
cpg	553.10	J/mol×K	782.20	Joback Method
cpg	565.20	J/mol×K	819.03	Joback Method
cpg	576.34	J/mol×K	855.85	Joback Method
cpg	586.55	J/mol×K	892.68	Joback Method
cpg	595.85	J/mol×K	929.50	Joback Method
cpg	604.27	J/mol×K	966.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299588&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