D-Alanine, N-(3-chloro-2-fluorobenzoyl)-, propyl ester

Inchi: InChI=1S/C13H15ClFNO3/c1-3-7-19-13(18)8(2)16-12(17)9-5-4-6-10(14)11(9)15/h4-6,8H

InchiKey: WLIDCKCRMJPHIE-UHFFFAOYSA-N

Formula: C13H15ClFNO3

SMILES: CCCOC(=O)C(C)NC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 287.71

Physical Properties

Property code	Value	Unit	Source
gf	-330.90	kJ/mol	Joback Method
hf	-619.10	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.551		Crippen Method
mcvol	203.270	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2026.00		NIST Webbook
rinpol	2026.00		NIST Webbook
tb	750.07	K	Joback Method
tc	960.15	K	Joback Method
tf	477.99	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.94	J/mol×K	750.07	Joback Method
cpg	558.14	J/mol×K	785.08	Joback Method
cpg	569.47	J/mol×K	820.10	Joback Method
cpg	579.96	J/mol×K	855.11	Joback Method
cpg	589.61	J/mol×K	890.13	Joback Method
cpg	598.45	J/mol×K	925.14	Joback Method
cpg	606.50	J/mol×K	960.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348334&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

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