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

Inchi: InChI=1S/C26H41ClFNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-32-26(31)21(2)29-

InchiKey: OGYBAKOGYAIDRE-UHFFFAOYSA-N

Formula: C26H41ClFNO3

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

Mol. weight [g/mol]: 470.06

Physical Properties

Property code	Value	Unit	Source
gf	-221.44	kJ/mol	Joback Method
hf	-887.42	kJ/mol	Joback Method
hfus	69.60	kJ/mol	Joback Method
hvap	102.59	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	7.622		Crippen Method
mcvol	386.440	ml/mol	McGowan Method
pc	883.14	kPa	Joback Method
rinpol	3348.00		NIST Webbook
tb	1047.51	K	Joback Method
tc	1287.57	K	Joback Method
tf	624.50	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.91	J/mol×K	1047.51	Joback Method
cpg	1323.20	J/mol×K	1087.52	Joback Method
cpg	1337.92	J/mol×K	1127.53	Joback Method
cpg	1351.15	J/mol×K	1167.54	Joback Method
cpg	1362.98	J/mol×K	1207.55	Joback Method
cpg	1373.49	J/mol×K	1247.56	Joback Method
cpg	1382.78	J/mol×K	1287.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348340&Units=SI

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