L-Valine, N-(3-chloro-2-fluorobenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C26H41ClFNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-32-26(31)24(20(2)3)29-

InchiKey: IDZJJGOBIMTAEJ-UHFFFAOYSA-N

Formula: C26H41ClFNO3

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

Mol. weight [g/mol]: 470.06

Physical Properties

Property code	Value	Unit	Source
gf	-223.88	kJ/mol	Joback Method
hf	-892.70	kJ/mol	Joback Method
hfus	66.08	kJ/mol	Joback Method
hvap	102.20	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.478		Crippen Method
mcvol	386.440	ml/mol	McGowan Method
pc	887.35	kPa	Joback Method
rinpol	3242.00		NIST Webbook
rinpol	3242.00		NIST Webbook
tb	1047.07	K	Joback Method
tc	1285.80	K	Joback Method
tf	609.50	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.15	J/mol×K	1047.07	Joback Method
cpg	1323.27	J/mol×K	1086.86	Joback Method
cpg	1337.82	J/mol×K	1126.65	Joback Method
cpg	1350.88	J/mol×K	1166.43	Joback Method
cpg	1362.53	J/mol×K	1206.22	Joback Method
cpg	1372.87	J/mol×K	1246.01	Joback Method
cpg	1381.97	J/mol×K	1285.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346546&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

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