L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C26H37F6NO3/c1-4-5-6-7-8-9-10-11-12-13-16-36-24(35)22(18(2)3)33-23(34)2

InchiKey: MTWXOSIINWAGKO-UHFFFAOYSA-N

Formula: C26H37F6NO3

SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 525.57

Physical Properties

Property code	Value	Unit	Source
gf	-1180.32	kJ/mol	Joback Method
hf	-1875.01	kJ/mol	Joback Method
hfus	62.45	kJ/mol	Joback Method
hvap	91.14	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	7.943		Crippen Method
mcvol	383.050	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	999.53	K	Joback Method
tc	1231.15	K	Joback Method
tf	587.37	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.74	J/mol×K	999.53	Joback Method
cpg	1332.76	J/mol×K	1038.13	Joback Method
cpg	1348.51	J/mol×K	1076.74	Joback Method
cpg	1363.12	J/mol×K	1115.34	Joback Method
cpg	1376.72	J/mol×K	1153.95	Joback Method
cpg	1389.44	J/mol×K	1192.55	Joback Method
cpg	1401.43	J/mol×K	1231.15	Joback Method

Sources

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=U346577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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