L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C25H37F4NO3/c1-4-5-6-7-8-9-10-11-12-13-17-33-24(32)22(18(2)3)30-23(31)1
InchiKey: VFEMLQLJNPWGAV-UHFFFAOYSA-N
Formula: C25H37F4NO3
SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C
Mol. weight [g/mol]: 475.56

Physical Properties

Property code	Value	Unit	Source
gf	-801.96	kJ/mol	Joback Method
hf	-1453.40	kJ/mol	Joback Method
hfus	61.11	kJ/mol	Joback Method
hvap	91.84	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	7.063		Crippen Method
mcvol	365.420	ml/mol	McGowan Method
pc	896.41	kPa	Joback Method
rinpol	2741.00		NIST Webbook
rinpol	2741.00		NIST Webbook
tb	981.34	K	Joback Method
tc	1203.96	K	Joback Method
tf	572.50	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.24	J/mol×K	981.34	Joback Method
cpg	1256.83	J/mol×K	1018.44	Joback Method
cpg	1272.09	J/mol×K	1055.55	Joback Method
cpg	1286.11	J/mol×K	1092.65	Joback Method
cpg	1298.98	J/mol×K	1129.75	Joback Method
cpg	1310.80	J/mol×K	1166.86	Joback Method
cpg	1321.64	J/mol×K	1203.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346473&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

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