L-Valine, N-(3-fluoro-4-trifluoromethylbenzoyl)-, decyl ester

Inchi: InChI=1S/C23H33F4NO3/c1-4-5-6-7-8-9-10-11-14-31-22(30)20(16(2)3)28-21(29)17-12-1

InchiKey: ZJUWKWRMVAAPJN-UHFFFAOYSA-N

Formula: C23H33F4NO3

SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1ccc(C(F)(F)F)c(F)c1)C(C)C

Mol. weight [g/mol]: 447.51

Physical Properties

Property code	Value	Unit	Source
gf	-818.80	kJ/mol	Joback Method
hf	-1412.12	kJ/mol	Joback Method
hfus	55.93	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.283		Crippen Method
mcvol	337.240	ml/mol	McGowan Method
pc	1009.09	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	935.58	K	Joback Method
tc	1145.43	K	Joback Method
tf	549.96	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.62	J/mol×K	935.58	Joback Method
cpg	1133.29	J/mol×K	970.56	Joback Method
cpg	1147.78	J/mol×K	1005.53	Joback Method
cpg	1161.16	J/mol×K	1040.51	Joback Method
cpg	1173.48	J/mol×K	1075.48	Joback Method
cpg	1184.83	J/mol×K	1110.46	Joback Method
cpg	1195.26	J/mol×K	1145.43	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=U346559&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

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