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

Inchi: InChI=1S/C21H29F4NO3/c1-4-5-6-7-8-9-13-29-20(28)18(14(2)3)26-19(27)15-11-10-12-1

InchiKey: LBGHIBAOKQEEHN-UHFFFAOYSA-N

Formula: C21H29F4NO3

SMILES: CCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C

Mol. weight [g/mol]: 419.45

Physical Properties

Property code	Value	Unit	Source
gf	-835.64	kJ/mol	Joback Method
hf	-1370.84	kJ/mol	Joback Method
hfus	50.75	kJ/mol	Joback Method
hvap	82.94	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.503		Crippen Method
mcvol	309.060	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	889.82	K	Joback Method
tc	1090.95	K	Joback Method
tf	527.42	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.33	J/mol×K	889.82	Joback Method
cpg	1012.24	J/mol×K	923.34	Joback Method
cpg	1026.08	J/mol×K	956.86	Joback Method
cpg	1038.89	J/mol×K	990.39	Joback Method
cpg	1050.74	J/mol×K	1023.91	Joback Method
cpg	1061.67	J/mol×K	1057.43	Joback Method
cpg	1071.74	J/mol×K	1090.95	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=U346469&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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