L-Valine, N-(2-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C14H16F3NO3/c1-8(2)11(13(20)21-3)18-12(19)9-6-4-5-7-10(9)14(15,16)17/h4

InchiKey: REAFSGAZPGLZFK-UHFFFAOYSA-N

Formula: C14H16F3NO3

SMILES: COC(=O)C(NC(=O)c1ccccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
hfus	29.93	kJ/mol	Joback Method
log10ws	-3.58		Cheméo Relay (1.0)
logp	2.633		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.19	J/mol×K	725.41	Joback Method
cpg	607.38	J/mol×K	758.90	Joback Method
cpg	619.63	J/mol×K	792.40	Joback Method
cpg	630.99	J/mol×K	825.89	Joback Method
cpg	641.50	J/mol×K	859.39	Joback Method
cpg	651.19	J/mol×K	892.88	Joback Method
cpg	660.12	J/mol×K	926.38	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299685&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices