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
gf	-690.14	kJ/mol	Joback Method
hf	-1018.78	kJ/mol	Joback Method
hfus	29.93	kJ/mol	Joback Method
hvap	67.51	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.633		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	725.41	K	Joback Method
tc	926.38	K	Joback Method
tf	435.42	K	Joback Method
vc	0.807	m3/kmol	Joback Method

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

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=U299685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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