L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C16H17F6NO3/c1-4-26-14(25)12(8(2)3)23-13(24)10-7-9(15(17,18)19)5-6-11(1

InchiKey: DHAMIGHWGJCHQG-UHFFFAOYSA-N

Formula: C16H17F6NO3

SMILES: CCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 385.30

Physical Properties

Property code	Value	Unit	Source
gf	-1264.52	kJ/mol	Joback Method
hf	-1668.61	kJ/mol	Joback Method
hfus	36.55	kJ/mol	Joback Method
hvap	68.88	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.042		Crippen Method
mcvol	242.150	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	770.73	K	Joback Method
tc	960.15	K	Joback Method
tf	474.67	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.93	J/mol×K	770.73	Joback Method
cpg	739.50	J/mol×K	802.30	Joback Method
cpg	751.18	J/mol×K	833.87	Joback Method
cpg	762.02	J/mol×K	865.44	Joback Method
cpg	772.08	J/mol×K	897.01	Joback Method
cpg	781.40	J/mol×K	928.58	Joback Method
cpg	790.04	J/mol×K	960.15	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=U346567&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