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

Inchi: InChI=1S/C14H17F2NO3/c1-4-20-14(19)12(8(2)3)17-13(18)10-7-9(15)5-6-11(10)16/h5-8
InchiKey: FKVQBAMMONGJND-UHFFFAOYSA-N
Formula: C14H17F2NO3
SMILES: CCOC(=O)C(NC(=O)c1cc(F)ccc1F)C(C)C
Mol. weight [g/mol]: 285.29

Physical Properties

Property code	Value	Unit	Source
gf	-507.80	kJ/mol	Joback Method
hf	-825.39	kJ/mol	Joback Method
hfus	33.88	kJ/mol	Joback Method
hvap	70.29	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.282		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	734.35	K	Joback Method
tc	934.70	K	Joback Method
tf	444.93	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.83	J/mol×K	734.35	Joback Method
cpg	596.16	J/mol×K	767.74	Joback Method
cpg	608.62	J/mol×K	801.13	Joback Method
cpg	620.22	J/mol×K	834.52	Joback Method
cpg	630.98	J/mol×K	867.92	Joback Method
cpg	640.91	J/mol×K	901.31	Joback Method
cpg	650.04	J/mol×K	934.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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