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

Inchi: InChI=1S/C17H23F2NO3/c1-4-5-6-9-23-17(22)15(11(2)3)20-16(21)13-10-12(18)7-8-14(1
InchiKey: LOEGLQBFJLZNDK-UHFFFAOYSA-N
Formula: C17H23F2NO3
SMILES: CCCCCOC(=O)C(NC(=O)c1cc(F)ccc1F)C(C)C
Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
gf	-482.54	kJ/mol	Joback Method
hf	-887.31	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	76.96	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.453		Crippen Method
mcvol	249.160	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	802.99	K	Joback Method
tc	1000.67	K	Joback Method
tf	478.74	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.67	J/mol×K	802.99	Joback Method
cpg	763.02	J/mol×K	835.94	Joback Method
cpg	776.39	J/mol×K	868.88	Joback Method
cpg	788.81	J/mol×K	901.83	Joback Method
cpg	800.30	J/mol×K	934.78	Joback Method
cpg	810.89	J/mol×K	967.72	Joback Method
cpg	820.60	J/mol×K	1000.67	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=U346457&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