L-Valine, N-(3,4-difluorobenzoyl)-, propyl ester

Inchi: InChI=1S/C15H19F2NO3/c1-4-7-21-15(20)13(9(2)3)18-14(19)10-5-6-11(16)12(17)8-10/h
InchiKey: MDBXFIUUFYBUJE-UHFFFAOYSA-N
Formula: C15H19F2NO3
SMILES: CCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1)C(C)C
Mol. weight [g/mol]: 299.31

Physical Properties

Property code	Value	Unit	Source
gf	-499.38	kJ/mol	Joback Method
hf	-846.03	kJ/mol	Joback Method
hfus	36.47	kJ/mol	Joback Method
hvap	72.51	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.672		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	757.23	K	Joback Method
tc	956.14	K	Joback Method
tf	456.20	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.06	J/mol×K	757.23	Joback Method
cpg	650.77	J/mol×K	790.38	Joback Method
cpg	663.57	J/mol×K	823.53	Joback Method
cpg	675.48	J/mol×K	856.68	Joback Method
cpg	686.53	J/mol×K	889.83	Joback Method
cpg	696.72	J/mol×K	922.99	Joback Method
cpg	706.08	J/mol×K	956.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346501&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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