L-Valine, N-(2,6-difluorobenzoyl)-, isohexyl ester

Inchi: InChI=1S/C18H25F2NO3/c1-11(2)7-6-10-24-18(23)16(12(3)4)21-17(22)15-13(19)8-5-9-1

InchiKey: NRXNYOZOTNWPFW-UHFFFAOYSA-N

Formula: C18H25F2NO3

SMILES: CC(C)CCCOC(=O)C(NC(=O)c1c(F)cccc1F)C(C)C

Mol. weight [g/mol]: 341.39

Physical Properties

Property code	Value	Unit	Source
gf	-476.56	kJ/mol	Joback Method
hf	-913.23	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.699		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	825.43	K	Joback Method
tc	1025.25	K	Joback Method
tf	475.01	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.43	J/mol×K	825.43	Joback Method
cpg	821.19	J/mol×K	858.73	Joback Method
cpg	834.91	J/mol×K	892.04	Joback Method
cpg	847.61	J/mol×K	925.34	Joback Method
cpg	859.33	J/mol×K	958.65	Joback Method
cpg	870.08	J/mol×K	991.95	Joback Method
cpg	879.91	J/mol×K	1025.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346618&Units=SI

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