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

Inchi: InChI=1S/C18H25F2NO3/c1-4-5-6-7-11-24-18(23)16(12(2)3)21-17(22)15-13(19)9-8-10-1
InchiKey: PURSPZPABDNROW-UHFFFAOYSA-N
Formula: C18H25F2NO3
SMILES: CCCCCCOC(=O)C(NC(=O)c1c(F)cccc1F)C(C)C
Mol. weight [g/mol]: 341.39

Physical Properties

Property code	Value	Unit	Source
gf	-474.12	kJ/mol	Joback Method
hf	-907.95	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	3.843		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	825.87	K	Joback Method
tc	1023.86	K	Joback Method
tf	490.01	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.88	J/mol×K	825.87	Joback Method
cpg	820.52	J/mol×K	858.87	Joback Method
cpg	834.14	J/mol×K	891.87	Joback Method
cpg	846.78	J/mol×K	924.86	Joback Method
cpg	858.45	J/mol×K	957.86	Joback Method
cpg	869.19	J/mol×K	990.86	Joback Method
cpg	879.03	J/mol×K	1023.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346619&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