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

Inchi: InChI=1S/C19H27F2NO3/c1-4-5-6-7-8-12-25-19(24)17(13(2)3)22-18(23)16-14(20)10-9-1
InchiKey: HBEBGDGXETWNHJ-UHFFFAOYSA-N
Formula: C19H27F2NO3
SMILES: CCCCCCCOC(=O)C(NC(=O)c1c(F)cccc1F)C(C)C
Mol. weight [g/mol]: 355.42

Physical Properties

Property code	Value	Unit	Source
gf	-465.70	kJ/mol	Joback Method
hf	-928.59	kJ/mol	Joback Method
hfus	46.83	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.233		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2373.00		NIST Webbook
rinpol	2373.00		NIST Webbook
tb	848.75	K	Joback Method
tc	1047.73	K	Joback Method
tf	501.28	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.95	J/mol×K	848.75	Joback Method
cpg	878.86	J/mol×K	881.91	Joback Method
cpg	892.72	J/mol×K	915.08	Joback Method
cpg	905.55	J/mol×K	948.24	Joback Method
cpg	917.38	J/mol×K	981.41	Joback Method
cpg	928.25	J/mol×K	1014.57	Joback Method
cpg	938.19	J/mol×K	1047.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346620&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