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

Inchi: InChI=1S/C20H29F2NO3/c1-4-5-6-7-8-9-12-26-20(25)18(14(2)3)23-19(24)15-10-11-16(2
InchiKey: BSAMHKZPUQVSLI-UHFFFAOYSA-N
Formula: C20H29F2NO3
SMILES: CCCCCCCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1)C(C)C
Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
gf	-457.28	kJ/mol	Joback Method
hf	-949.23	kJ/mol	Joback Method
hfus	49.42	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.623		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	871.63	K	Joback Method
tc	1072.35	K	Joback Method
tf	512.55	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.80	J/mol×K	871.63	Joback Method
cpg	937.99	J/mol×K	905.08	Joback Method
cpg	952.07	J/mol×K	938.54	Joback Method
cpg	965.09	J/mol×K	971.99	Joback Method
cpg	977.07	J/mol×K	1005.44	Joback Method
cpg	988.05	J/mol×K	1038.89	Joback Method
cpg	998.06	J/mol×K	1072.35	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=U346505&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