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

Inchi: InChI=1S/C26H41F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-32-26(31)24(20(2)3)29-2

InchiKey: GTWNASFRWBBCGR-UHFFFAOYSA-N

Formula: C26H41F2NO3

SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)cccc1F)C(C)C

Mol. weight [g/mol]: 453.61

Physical Properties

Property code	Value	Unit	Source
gf	-406.76	kJ/mol	Joback Method
hf	-1073.07	kJ/mol	Joback Method
hfus	64.96	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-8.75		Crippen Method
logp	6.964		Crippen Method
mcvol	375.970	ml/mol	McGowan Method
pc	883.14	kPa	Joback Method
rinpol	3107.00		NIST Webbook
rinpol	3107.00		NIST Webbook
tb	1008.91	K	Joback Method
tc	1239.03	K	Joback Method
tf	580.17	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.96	J/mol×K	1008.91	Joback Method
cpg	1306.15	J/mol×K	1047.26	Joback Method
cpg	1321.79	J/mol×K	1085.62	Joback Method
cpg	1335.93	J/mol×K	1123.97	Joback Method
cpg	1348.67	J/mol×K	1162.32	Joback Method
cpg	1360.07	J/mol×K	1200.67	Joback Method
cpg	1370.21	J/mol×K	1239.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346624&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