L-Valine, N-(2,5-difluorobenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C29H47F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-35-29(34)27(23
InchiKey: OTUSXEJIGQYRAI-UHFFFAOYSA-N
Formula: C29H47F2NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)ccc1F)C(C)C
Mol. weight [g/mol]: 495.69

Physical Properties

Property code	Value	Unit	Source
gf	-381.50	kJ/mol	Joback Method
hf	-1134.99	kJ/mol	Joback Method
hfus	72.73	kJ/mol	Joback Method
hvap	103.68	kJ/mol	Joback Method
log10ws	-10.00		Crippen Method
logp	8.134		Crippen Method
mcvol	418.240	ml/mol	McGowan Method
pc	749.38	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1077.55	K	Joback Method
tc	1337.98	K	Joback Method
tf	613.98	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1478.17	J/mol×K	1077.55	Joback Method
cpg	1496.84	J/mol×K	1120.95	Joback Method
cpg	1513.53	J/mol×K	1164.36	Joback Method
cpg	1528.36	J/mol×K	1207.76	Joback Method
cpg	1541.48	J/mol×K	1251.17	Joback Method
cpg	1552.99	J/mol×K	1294.57	Joback Method
cpg	1563.03	J/mol×K	1337.98	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=U346462&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