L-Valine, N-(3-methoxy-2,4,5-trifluorobenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C30H48F3NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-38-30(36)27(2
Inchikey: QTZHQVKVSKZRQG-UHFFFAOYSA-N
Formula: C30H48F3NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 543.70

Physical Properties

Property code	Value	Unit	Source
gf	-692.15	kJ/mol	Joback Method
hf	-1506.90	kJ/mol	Joback Method
hfus	78.81	kJ/mol	Joback Method
hvap	108.82	kJ/mol	Joback Method
log10ws	-10.45		Crippen Method
logp	8.281		Crippen Method
mcvol	439.970	ml/mol	McGowan Method
pc	677.82	kPa	Joback Method
rinpol	3473.00		NIST Webbook
rinpol	3473.00		NIST Webbook
tb	1132.08	K	Joback Method
tc	1431.53	K	Joback Method
tf	673.11	K	Joback Method
vc	1.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.23	J/mol×K	1132.08	Joback Method
cpg	1589.60	J/mol×K	1181.99	Joback Method
cpg	1603.93	J/mol×K	1231.90	Joback Method
cpg	1615.33	J/mol×K	1281.80	Joback Method
cpg	1623.94	J/mol×K	1331.71	Joback Method
cpg	1629.88	J/mol×K	1381.62	Joback Method
cpg	1633.28	J/mol×K	1431.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346441&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

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