L-Valine, N-(2-fluoro-6-trifluoromethylbenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H43F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-36-27(35)25(21(2)3)3
InchiKey: DRSPFBGGLRRRJS-UHFFFAOYSA-N
Formula: C28H43F4NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)cccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 517.64

Physical Properties

Property code	Value	Unit	Source
gf	-776.70	kJ/mol	Joback Method
hf	-1515.32	kJ/mol	Joback Method
hfus	68.88	kJ/mol	Joback Method
hvap	98.52	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.233		Crippen Method
mcvol	407.690	ml/mol	McGowan Method
pc	759.74	kPa	Joback Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook
tb	1049.98	K	Joback Method
tc	1300.80	K	Joback Method
tf	606.31	K	Joback Method
vc	1.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.80	J/mol×K	1049.98	Joback Method
cpg	1446.15	J/mol×K	1091.78	Joback Method
cpg	1462.88	J/mol×K	1133.59	Joback Method
cpg	1478.14	J/mol×K	1175.39	Joback Method
cpg	1492.05	J/mol×K	1217.19	Joback Method
cpg	1504.78	J/mol×K	1258.99	Joback Method
cpg	1516.46	J/mol×K	1300.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346496&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

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