L-Valine, N-(5-fluoro-2-trifluoromethyl)-, octadecyl ester

Inchi: InChI=1S/C31H49F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-39-30(38)28
InchiKey: XKZWYJAYBYIJNH-UHFFFAOYSA-N
Formula: C31H49F4NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 559.72

Physical Properties

Property code	Value	Unit	Source
gf	-751.44	kJ/mol	Joback Method
hf	-1577.24	kJ/mol	Joback Method
hfus	76.65	kJ/mol	Joback Method
hvap	105.20	kJ/mol	Joback Method
log10ws	-11.19		Crippen Method
logp	9.404		Crippen Method
mcvol	449.960	ml/mol	McGowan Method
pc	652.10	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook
tb	1118.62	K	Joback Method
tc	1410.90	K	Joback Method
tf	640.12	K	Joback Method
vc	1.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.91	J/mol×K	1118.62	Joback Method
cpg	1639.67	J/mol×K	1167.33	Joback Method
cpg	1658.40	J/mol×K	1216.05	Joback Method
cpg	1675.35	J/mol×K	1264.76	Joback Method
cpg	1690.78	J/mol×K	1313.47	Joback Method
cpg	1704.93	J/mol×K	1362.18	Joback Method
cpg	1718.07	J/mol×K	1410.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346431&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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