L-Valine, N-(3-trifluoromethylbenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C29H46F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-36-28(35)26(23(2)
InchiKey: FWZNEBJOUCJOAL-UHFFFAOYSA-N
Formula: C29H46F3NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C
Mol. weight [g/mol]: 513.68

Physical Properties

Property code	Value	Unit	Source
gf	-563.84	kJ/mol	Joback Method
hf	-1328.38	kJ/mol	Joback Method
hfus	68.78	kJ/mol	Joback Method
hvap	100.90	kJ/mol	Joback Method
log10ws	-10.02		Crippen Method
logp	8.484		Crippen Method
mcvol	420.010	ml/mol	McGowan Method
pc	744.88	kPa	Joback Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook
tb	1068.61	K	Joback Method
tc	1324.43	K	Joback Method
tf	604.47	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1485.50	J/mol×K	1068.61	Joback Method
cpg	1504.51	J/mol×K	1111.25	Joback Method
cpg	1521.90	J/mol×K	1153.88	Joback Method
cpg	1537.84	J/mol×K	1196.52	Joback Method
cpg	1552.49	J/mol×K	1239.16	Joback Method
cpg	1566.01	J/mol×K	1281.79	Joback Method
cpg	1578.59	J/mol×K	1324.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346728&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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