L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C29H43F6NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-39-27(38)25(21(2)3)3

InchiKey: SQKBFHOEZFKWDV-UHFFFAOYSA-N

Formula: C29H43F6NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 567.65

Physical Properties

Property code	Value	Unit	Source
gf	-1155.06	kJ/mol	Joback Method
hf	-1936.93	kJ/mol	Joback Method
hfus	70.22	kJ/mol	Joback Method
hvap	97.82	kJ/mol	Joback Method
log10ws	-10.71		Crippen Method
logp	9.113		Crippen Method
mcvol	425.320	ml/mol	McGowan Method
pc	694.35	kPa	Joback Method
rinpol	2913.00		NIST Webbook
rinpol	2913.00		NIST Webbook
tb	1068.17	K	Joback Method
tc	1334.08	K	Joback Method
tf	621.18	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1504.12	J/mol×K	1068.17	Joback Method
cpg	1523.58	J/mol×K	1112.49	Joback Method
cpg	1541.52	J/mol×K	1156.81	Joback Method
cpg	1558.17	J/mol×K	1201.13	Joback Method
cpg	1573.75	J/mol×K	1245.45	Joback Method
cpg	1588.47	J/mol×K	1289.76	Joback Method
cpg	1602.57	J/mol×K	1334.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346579&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