l-Valine, n-heptafluorobutyryl-, octadecyl ester

Inchi: InChI=1S/C27H46F7NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-38-23(36)22
InchiKey: ZPMIUNZCRHHDPP-UHFFFAOYSA-N
Formula: C27H46F7NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 565.65

Physical Properties

Property code	Value	Unit	Source
gf	-1457.02	kJ/mol	Joback Method
hf	-2314.10	kJ/mol	Joback Method
hfus	67.44	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	8.765		Crippen Method
mcvol	422.670	ml/mol	McGowan Method
pc	647.46	kPa	Joback Method
rinpol	2636.00		NIST Webbook
tb	981.81	K	Joback Method
tc	1229.03	K	Joback Method
tf	550.19	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.72	J/mol×K	981.81	Joback Method
cpg	1512.84	J/mol×K	1023.01	Joback Method
cpg	1533.46	J/mol×K	1064.22	Joback Method
cpg	1552.79	J/mol×K	1105.42	Joback Method
cpg	1571.03	J/mol×K	1146.62	Joback Method
cpg	1588.41	J/mol×K	1187.83	Joback Method
cpg	1605.12	J/mol×K	1229.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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