l-Valine, n-heptafluorobutyryl-, pentadecyl ester

Inchi: InChI=1S/C24H40F7NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-35-20(33)19(18(2)3)3

InchiKey: CDUBMNUSBILHGR-UHFFFAOYSA-N

Formula: C24H40F7NO3

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

Mol. weight [g/mol]: 523.57

Physical Properties

Property code	Value	Unit	Source
gf	-1482.28	kJ/mol	Joback Method
hf	-2252.18	kJ/mol	Joback Method
hfus	59.67	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	7.594		Crippen Method
mcvol	380.400	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	2351.00		NIST Webbook
rinpol	2351.00		NIST Webbook
tb	913.17	K	Joback Method
tc	1126.22	K	Joback Method
tf	516.38	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.35	J/mol×K	913.17	Joback Method
cpg	1320.46	J/mol×K	948.68	Joback Method
cpg	1338.32	J/mol×K	984.19	Joback Method
cpg	1355.07	J/mol×K	1019.69	Joback Method
cpg	1370.83	J/mol×K	1055.20	Joback Method
cpg	1385.72	J/mol×K	1090.71	Joback Method
cpg	1399.87	J/mol×K	1126.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320905&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