L-Valine, N-pentafluorobenzoyl-, tetradecyl ester

Inchi: InChI=1S/C26H38F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-35-26(34)24(17(2)3)32-2

InchiKey: MXYLGPFZTACMFT-UHFFFAOYSA-N

Formula: C26H38F5NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 507.58

Physical Properties

Property code	Value	Unit	Source
gf	-1020.08	kJ/mol	Joback Method
hf	-1695.81	kJ/mol	Joback Method
hfus	73.03	kJ/mol	Joback Method
hvap	96.53	kJ/mol	Joback Method
log10ws	-9.74		Crippen Method
logp	7.381		Crippen Method
mcvol	381.280	ml/mol	McGowan Method
pc	795.73	kPa	Joback Method
rinpol	2863.00		NIST Webbook
rinpol	2863.00		NIST Webbook
tb	1021.66	K	Joback Method
tc	1266.90	K	Joback Method
tf	619.50	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.65	J/mol×K	1021.66	Joback Method
cpg	1323.74	J/mol×K	1062.53	Joback Method
cpg	1338.98	J/mol×K	1103.41	Joback Method
cpg	1352.44	J/mol×K	1144.28	Joback Method
cpg	1364.19	J/mol×K	1185.16	Joback Method
cpg	1374.29	J/mol×K	1226.03	Joback Method
cpg	1382.82	J/mol×K	1266.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346613&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