L-Valine, N-heptafluorobutyryl-, hexadecyl ester

Inchi: InChI=1S/C25H42F7NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-36-21(34)20(19(2)
InchiKey: NXGNMICEPSUWMX-UHFFFAOYSA-N
Formula: C25H42F7NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 537.60

Physical Properties

Property code	Value	Unit	Source
hfus	62.26	kJ/mol	Joback Method
log10ws	-8.31		Cheméo Relay (1.0)
logp	7.985		Crippen Method
mcvol	394.490	ml/mol	McGowan Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	613.89	K	Cheméo Relay (1.0)
tf	342.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.92	J/mol×K	936.05	Joback Method
cpg	1383.93	J/mol×K	973.23	Joback Method
cpg	1402.61	J/mol×K	1010.41	Joback Method
cpg	1420.12	J/mol×K	1047.59	Joback Method
cpg	1436.61	J/mol×K	1084.76	Joback Method
cpg	1452.21	J/mol×K	1121.94	Joback Method
cpg	1467.09	J/mol×K	1159.12	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320906&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point