L-Leucine, N-heptafluorobutyryl-, octadecyl ester

Inchi: InChI=1S/C28H48F7NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-39-24(37)23

InchiKey: CLFVCIUIGNNHON-UHFFFAOYSA-N

Formula: C28H48F7NO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 579.68

Physical Properties

Property code	Value	Unit	Source
hfus	70.03	kJ/mol	Joback Method
log10ws	-9.10		Cheméo Relay (1.0)
logp	9.155		Crippen Method
mcvol	436.760	ml/mol	McGowan Method
rinpol	2684.00		NIST Webbook
tb	648.25	K	Cheméo Relay (1.0)
tf	335.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.90	J/mol×K	1004.69	Joback Method
cpg	1578.26	J/mol×K	1048.29	Joback Method
cpg	1600.02	J/mol×K	1091.88	Joback Method
cpg	1620.44	J/mol×K	1135.48	Joback Method
cpg	1639.76	J/mol×K	1179.07	Joback Method
cpg	1658.25	J/mol×K	1222.67	Joback Method
cpg	1676.16	J/mol×K	1266.27	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321004&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

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