L-Leucine, N-pentafluoropropionyl-, propyl ester

Inchi: InChI=1S/C12H18F5NO3/c1-4-5-21-9(19)8(6-7(2)3)18-10(20)11(13,14)12(15,16)17/h7-8
InchiKey: LSASGAMACFKGEV-UHFFFAOYSA-N
Formula: C12H18F5NO3
SMILES: CCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
hfus	29.85	kJ/mol	Joback Method
logp	2.668		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
tb	487.80	K	Cheméo Relay (1.0)
tc	622.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.84	J/mol×K	643.30	Joback Method
cpg	604.14	J/mol×K	671.57	Joback Method
cpg	616.68	J/mol×K	699.83	Joback Method
cpg	628.49	J/mol×K	728.10	Joback Method
cpg	639.60	J/mol×K	756.37	Joback Method
cpg	650.05	J/mol×K	784.63	Joback Method
cpg	659.86	J/mol×K	812.90	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=U321006&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
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

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