

L-Leucine, N-heptafluorobutyryl-, butyl ester

Inchi:	InChI=1S/C14H20F7NO3/c1-4-5-6-25-10(23)9(7-8(2)3)22-11(24)12(15,16)13(17,18)14(19)20
InchiKey:	DQNQXBWJRDSSEK-UHFFFAOYSA-N
Formula:	C14H20F7NO3
SMILES:	CCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	383.30

Physical Properties

Property code	Value	Unit	Source
hfus	33.77	kJ/mol	Joback Method
logp	3.693		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
tb	507.27	K	Cheméo Relay (1.0)
tf	284.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.56	J/mol×K	684.37	Joback Method
cpg	729.16	J/mol×K	712.12	Joback Method
cpg	741.94	J/mol×K	739.87	Joback Method
cpg	753.94	J/mol×K	767.61	Joback Method
cpg	765.22	J/mol×K	795.36	Joback Method
cpg	775.80	J/mol×K	823.11	Joback Method
cpg	785.74	J/mol×K	850.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U320992&Units=SI>

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
hfus:	Enthalpy of fusion at standard conditions
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

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