

I-Leucine, n-heptafluorobutyryl-, heptyl ester

Inchi:	InChI=1S/C17H26F7NO3/c1-4-5-6-7-8-9-28-13(26)12(10-11(2)3)25-14(27)15(18,19)16(2
InchiKey:	MZGMHEOMBKWFCT-UHFFFAOYSA-N
Formula:	C17H26F7NO3
SMILES:	CCCCCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	425.38

Physical Properties

Property code	Value	Unit	Source
gf	-1541.22	kJ/mol	Joback Method
hf	-2107.70	kJ/mol	Joback Method
hfus	41.54	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.864		Crippen Method
mvol	281.770	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rmpol	1654.00		NIST Webbook
rmpol	1654.00		NIST Webbook
tb	753.01	K	Joback Method
tc	925.32	K	Joback Method
tf	437.49	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.31	J/molxK	753.01	Joback Method
cpg	897.16	J/molxK	781.73	Joback Method
cpg	911.11	J/molxK	810.45	Joback Method
cpg	924.23	J/molxK	839.17	Joback Method
cpg	936.57	J/molxK	867.88	Joback Method
cpg	948.18	J/molxK	896.60	Joback Method
cpg	959.11	J/molxK	925.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320996&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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