L-Isoleucine, N-heptafluorobutyryl-, heptyl ester

Inchi: InChI=1S/C17H26F7NO3/c1-4-6-7-8-9-10-28-13(26)12(11(3)5-2)25-14(27)15(18,19)16(2

InchiKey: YZXBJVKQDRIDBH-UHFFFAOYSA-N

Formula: C17H26F7NO3

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

Mol. weight [g/mol]: 425.38

Physical Properties

Property code	Value	Unit	Source
hfus	41.54	kJ/mol	Joback Method
log10ws	-5.99		Cheméo Relay (1.0)
logp	4.864		Crippen Method
mcvol	281.770	ml/mol	McGowan Method
rinpol	1667.00		NIST Webbook
tb	539.66	K	Cheméo Relay (1.0)
tf	297.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320926&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