L-Isoleucine, N-heptafluorobutyryl-, octyl ester

Inchi: InChI=1S/C18H28F7NO3/c1-4-6-7-8-9-10-11-29-14(27)13(12(3)5-2)26-15(28)16(19,20)1
InchiKey: VIRRLCOMTMVYSF-UHFFFAOYSA-N
Formula: C18H28F7NO3
SMILES: CCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)CC
Mol. weight [g/mol]: 439.41

Physical Properties

Property code	Value	Unit	Source
hfus	44.13	kJ/mol	Joback Method
log10ws	-6.31		Cheméo Relay (1.0)
logp	5.254		Crippen Method
mcvol	295.860	ml/mol	McGowan Method
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
tb	551.10	K	Cheméo Relay (1.0)
tf	301.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.82	J/mol×K	775.89	Joback Method
cpg	955.13	J/mol×K	805.15	Joback Method
cpg	969.51	J/mol×K	834.40	Joback Method
cpg	983.03	J/mol×K	863.66	Joback Method
cpg	995.74	J/mol×K	892.91	Joback Method
cpg	1007.71	J/mol×K	922.17	Joback Method
cpg	1018.99	J/mol×K	951.43	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=U320927&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