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
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
mcvol	281.770	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	1667.00		NIST Webbook
tb	753.01	K	Joback Method
tc	925.32	K	Joback Method
tf	437.49	K	Joback Method
vc	1.133	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320926&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume