L-Isoleucine, N-pentafluoropropionyl-, heptyl ester

Inchi: InChI=1S/C16H26F5NO3/c1-4-6-7-8-9-10-25-13(23)12(11(3)5-2)22-14(24)15(17,18)16(1

InchiKey: JOXLPJIXSVEXKP-UHFFFAOYSA-N

Formula: C16H26F5NO3

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

Mol. weight [g/mol]: 375.38

Physical Properties

Property code	Value	Unit	Source
hf	-1855.79	kJ/mol	Cheméo Relay (1.0)
hfus	40.21	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.30		Cheméo Relay (1.0)
logp	4.228		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	530.48	K	Cheméo Relay (1.0)
tf	310.24	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.18	J/mol×K	734.82	Joback Method
cpg	823.18	J/mol×K	763.59	Joback Method
cpg	837.32	J/mol×K	792.36	Joback Method
cpg	850.64	J/mol×K	821.13	Joback Method
cpg	863.18	J/mol×K	849.90	Joback Method
cpg	874.98	J/mol×K	878.68	Joback Method
cpg	886.09	J/mol×K	907.45	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=U320869&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point