

I-Isoleucine, n-heptafluorobutyryl-, heptadecyl ester

Inchi:	InChI=1S/C27H46F7NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-38-23(36)22(
InchiKey:	PEIJALRGLVZUNZ-UHFFFAOYSA-N
Formula:	C27H46F7NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(C)CC
Mol. weight [g/mol]:	565.65

Physical Properties

Property code	Value	Unit	Source
gf	-1457.02	kJ/mol	Joback Method
hf	-2314.10	kJ/mol	Joback Method
hfus	67.44	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	8.765		Crippen Method
mvol	422.670	ml/mol	McGowan Method
pc	647.46	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2602.00		NIST Webbook
tb	981.81	K	Joback Method
tc	1229.03	K	Joback Method
tf	550.19	K	Joback Method
vc	1.694	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.72	J/molxK	981.81	Joback Method
cpg	1512.84	J/molxK	1023.01	Joback Method
cpg	1533.46	J/molxK	1064.22	Joback Method
cpg	1552.79	J/molxK	1105.42	Joback Method
cpg	1571.03	J/molxK	1146.62	Joback Method
cpg	1588.41	J/molxK	1187.83	Joback Method
cpg	1605.12	J/molxK	1229.03	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=U320934&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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