

I-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]:	375.37

Physical Properties

Property code	Value	Unit	Source
gf	-1162.86	kJ/mol	Joback Method
hf	-1686.09	kJ/mol	Joback Method
hfus	40.21	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.228		Crippen Method
mvol	264.140	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	734.82	K	Joback Method
tc	907.45	K	Joback Method
tf	422.62	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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