

I-Isoleucine, n-heptafluorobutyryl-, octadecyl ester

Inchi:	InChI=1S/C28H48F7NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-39-24(37)
InchiKey:	QNJII SAOUXOCTE-UHFFFAOYSA-N
Formula:	C28H48F7NO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(C)CC
Mol. weight [g/mol]:	579.67

Physical Properties

Property code	Value	Unit	Source
gf	-1448.60	kJ/mol	Joback Method
hf	-2334.74	kJ/mol	Joback Method
hfus	70.03	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-10.53		Crippen Method
logp	9.155		Crippen Method
mcvol	436.760	ml/mol	McGowan Method
pc	616.95	kPa	Joback Method
rinpola	2704.00		NIST Webbook
rinpola	2704.00		NIST Webbook
tb	1004.69	K	Joback Method
tc	1266.27	K	Joback Method
tf	561.46	K	Joback Method
vc	1.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.90	J/molxK	1004.69	Joback Method
cpg	1578.26	J/molxK	1048.29	Joback Method
cpg	1600.02	J/molxK	1091.88	Joback Method
cpg	1620.44	J/molxK	1135.48	Joback Method
cpg	1639.76	J/molxK	1179.07	Joback Method
cpg	1658.25	J/molxK	1222.67	Joback Method
cpg	1676.16	J/molxK	1266.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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