

I-Isoleucine, n-heptafluorobutyryl-, tetradecyl ester

Inchi:	InChI=1S/C24H40F7NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-35-20(33)19(18(3)5-2)3
InchiKey:	HPFBDSQMGMVUDO-UHFFFAOYSA-N
Formula:	C24H40F7NO3
SMILES:	CCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(C)CC
Mol. weight [g/mol]:	523.57

Physical Properties

Property code	Value	Unit	Source
gf	-1482.28	kJ/mol	Joback Method
hf	-2252.18	kJ/mol	Joback Method
hfus	59.67	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	7.594		Crippen Method
mvol	380.400	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	913.17	K	Joback Method
tc	1126.22	K	Joback Method
tf	516.38	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.35	J/molxK	913.17	Joback Method
cpg	1320.46	J/molxK	948.68	Joback Method
cpg	1338.32	J/molxK	984.19	Joback Method
cpg	1355.07	J/molxK	1019.69	Joback Method
cpg	1370.83	J/molxK	1055.20	Joback Method
cpg	1385.72	J/molxK	1090.71	Joback Method
cpg	1399.87	J/molxK	1126.22	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=U320931&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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