L-Methionine, N-pentafluoropropionyl-, isohexyl ester

Inchi: InChI=1S/C14H22F5NO3S/c1-9(2)5-4-7-23-11(21)10(6-8-24-3)20-12(22)13(15,16)14(17

InchiKey: ZGCRHFLMSIWKGO-UHFFFAOYSA-N

Formula: C14H22F5NO3S

SMILES: CSCCC(NC(=O)C(F)(F)C(F)(F)F)C(=O)OCCCC(C)C

Mol. weight [g/mol]: 379.39

Physical Properties

Property code	Value	Unit	Source
hfus	39.16	kJ/mol	Joback Method
logp	3.401		Crippen Method
mcvol	252.310	ml/mol	McGowan Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.63	J/mol×K	757.84	Joback Method
cpg	770.08	J/mol×K	788.48	Joback Method
cpg	782.65	J/mol×K	819.13	Joback Method
cpg	794.37	J/mol×K	849.77	Joback Method
cpg	805.29	J/mol×K	880.42	Joback Method
cpg	815.45	J/mol×K	911.06	Joback Method
cpg	824.88	J/mol×K	941.71	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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=U320913&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices