L-Methionine, N-heptafluorobutyryl-, pentadecyl ester

Inchi: InChI=1S/C24H40F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-17-35-20(33)19(16-18-3

InchiKey: DGPJRLNCMSOIIK-UHFFFAOYSA-N

Formula: C24H40F7NO3S

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 555.64

Physical Properties

Property code	Value	Unit	Source
hfus	67.33	kJ/mol	Joback Method
logp	7.692		Crippen Method
mcvol	396.750	ml/mol	McGowan Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	653.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.59	J/mol×K	982.39	Joback Method
cpg	1381.77	J/mol×K	1021.42	Joback Method
cpg	1398.63	J/mol×K	1060.46	Joback Method
cpg	1414.34	J/mol×K	1099.49	Joback Method
cpg	1429.05	J/mol×K	1138.52	Joback Method
cpg	1442.91	J/mol×K	1177.56	Joback Method
cpg	1456.09	J/mol×K	1216.59	Joback Method

Sources

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=U320861&Units=SI

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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature