L-Methionine, N-pentafluoropropionyl-, pentadecyl ester

Inchi: InChI=1S/C23H40F5NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-17-32-20(30)19(16-18-3

InchiKey: XSCFPCVGWDCWRC-UHFFFAOYSA-N

Formula: C23H40F5NO3S

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

Mol. weight [g/mol]: 505.63

Physical Properties

Property code	Value	Unit	Source
hfus	65.99	kJ/mol	Joback Method
logp	7.056		Crippen Method
mcvol	379.120	ml/mol	McGowan Method
rinpol	2671.00		NIST Webbook
tb	642.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.81	J/mol×K	964.20	Joback Method
cpg	1305.38	J/mol×K	1001.35	Joback Method
cpg	1321.61	J/mol×K	1038.50	Joback Method
cpg	1336.62	J/mol×K	1075.65	Joback Method
cpg	1350.50	J/mol×K	1112.80	Joback Method
cpg	1363.37	J/mol×K	1149.94	Joback Method
cpg	1375.32	J/mol×K	1187.09	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=U320922&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