L-Methionine, N-heptafluorobutyryl-, butyl ester

Inchi: InChI=1S/C13H18F7NO3S/c1-3-4-6-24-9(22)8(5-7-25-2)21-10(23)11(14,15)12(16,17)13(

InchiKey: RAYWSDPQZFLTFJ-UHFFFAOYSA-N

Formula: C13H18F7NO3S

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

Mol. weight [g/mol]: 401.34

Physical Properties

Property code	Value	Unit	Source
hfus	38.84	kJ/mol	Joback Method
logp	3.401		Crippen Method
mcvol	241.760	ml/mol	McGowan Method
rinpol	1631.00		NIST Webbook
tb	543.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.16	J/mol×K	730.71	Joback Method
cpg	731.45	J/mol×K	760.32	Joback Method
cpg	742.91	J/mol×K	789.94	Joback Method
cpg	753.58	J/mol×K	819.55	Joback Method
cpg	763.52	J/mol×K	849.17	Joback Method
cpg	772.77	J/mol×K	878.78	Joback Method
cpg	781.38	J/mol×K	908.40	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=U320852&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