L-Methionine, N-heptafluorobutyryl-, isobutyl ester

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

InchiKey: YOFLPQABMWTVEW-UHFFFAOYSA-N

Formula: C13H18F7NO3S

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

Mol. weight [g/mol]: 401.34

Physical Properties

Property code	Value	Unit	Source
hfus	35.31	kJ/mol	Joback Method
logp	3.256		Crippen Method
mcvol	241.760	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.72	J/mol×K	730.27	Joback Method
cpg	732.15	J/mol×K	760.18	Joback Method
cpg	743.72	J/mol×K	790.10	Joback Method
cpg	754.49	J/mol×K	820.01	Joback Method
cpg	764.49	J/mol×K	849.92	Joback Method
cpg	773.79	J/mol×K	879.84	Joback Method
cpg	782.43	J/mol×K	909.75	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320851&Units=SI

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):

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