L-Methionine, N-(2-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C14H16F3NO3S/c1-21-13(20)11(7-8-22-2)18-12(19)9-5-3-4-6-10(9)14(15,16)1

InchiKey: RVQXGMNGQXKZSU-UHFFFAOYSA-N

Formula: C14H16F3NO3S

SMILES: COC(=O)C(CCSC)NC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 335.35

Physical Properties

Property code	Value	Unit	Source
hfus	37.59	kJ/mol	Joback Method
logp	2.730		Crippen Method
mcvol	225.010	ml/mol	McGowan Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.34	J/mol×K	794.63	Joback Method
cpg	658.40	J/mol×K	829.89	Joback Method
cpg	669.46	J/mol×K	865.15	Joback Method
cpg	679.57	J/mol×K	900.41	Joback Method
cpg	688.75	J/mol×K	935.67	Joback Method
cpg	697.06	J/mol×K	970.93	Joback Method
cpg	704.52	J/mol×K	1006.18	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=U299687&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