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]: 335.34

Physical Properties

Property code	Value	Unit	Source
gf	-654.58	kJ/mol	Joback Method
hf	-971.63	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.730		Crippen Method
mcvol	225.010	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	794.63	K	Joback Method
tc	1006.18	K	Joback Method
tf	484.82	K	Joback Method
vc	0.868	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume