l-Methionine, N-(4-fluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H16FNO3S/c1-18-13(17)11(7-8-19-2)15-12(16)9-3-5-10(14)6-4-9/h3-6,11H

InchiKey: QWBCYKWKXNQPRH-UHFFFAOYSA-N

Formula: C13H16FNO3S

SMILES: COC(=O)C(CCSC)NC(=O)c1ccc(F)cc1

Mol. weight [g/mol]: 285.33

Physical Properties

Property code	Value	Unit	Source
gf	-276.22	kJ/mol	Joback Method
hf	-550.02	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.850		Crippen Method
mcvol	207.380	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2093.00		NIST Webbook
tb	776.44	K	Joback Method
tc	996.20	K	Joback Method
tf	469.95	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.82	J/mol×K	776.44	Joback Method
cpg	587.42	J/mol×K	813.07	Joback Method
cpg	598.99	J/mol×K	849.69	Joback Method
cpg	609.54	J/mol×K	886.32	Joback Method
cpg	619.11	J/mol×K	922.95	Joback Method
cpg	627.70	J/mol×K	959.57	Joback Method
cpg	635.33	J/mol×K	996.20	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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