l-Methionine, N-(p-anisoyl)-, methyl ester

Inchi: InChI=1S/C14H19NO4S/c1-18-11-6-4-10(5-7-11)13(16)15-12(8-9-20-3)14(17)19-2/h4-7,
InchiKey: NJDQZPBLHXZZEQ-UHFFFAOYSA-N
Formula: C14H19NO4S
SMILES: COC(=O)C(CCSC)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 297.37

Physical Properties

Property code	Value	Unit	Source
gf	-177.99	kJ/mol	Joback Method
hf	-506.77	kJ/mol	Joback Method
hfus	36.95	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	1.720		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	822.47	K	Joback Method
tc	1045.51	K	Joback Method
tf	502.86	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.85	J/mol×K	822.47	Joback Method
cpg	660.80	J/mol×K	859.64	Joback Method
cpg	672.57	J/mol×K	896.82	Joback Method
cpg	683.16	J/mol×K	933.99	Joback Method
cpg	692.59	J/mol×K	971.16	Joback Method
cpg	700.84	J/mol×K	1008.34	Joback Method
cpg	707.93	J/mol×K	1045.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299672&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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