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

Inchi: InChI=1S/C13H16BrNO3S/c1-18-13(17)11(7-8-19-2)15-12(16)9-3-5-10(14)6-4-9/h3-6,11

InchiKey: SAJBRQJWHODIEA-UHFFFAOYSA-N

Formula: C13H16BrNO3S

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

Mol. weight [g/mol]: 346.24

Physical Properties

Property code	Value	Unit	Source
gf	-67.09	kJ/mol	Joback Method
hf	-327.58	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.474		Crippen Method
mcvol	223.110	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	843.33	K	Joback Method
tc	1080.85	K	Joback Method
tf	529.16	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.39	J/mol×K	843.33	Joback Method
cpg	610.75	J/mol×K	882.92	Joback Method
cpg	621.02	J/mol×K	922.50	Joback Method
cpg	630.22	J/mol×K	962.09	Joback Method
cpg	638.40	J/mol×K	1001.68	Joback Method
cpg	645.57	J/mol×K	1041.26	Joback Method
cpg	651.78	J/mol×K	1080.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299617&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