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

Inchi: InChI=1S/C17H25NO3S/c1-4-5-6-13-7-9-14(10-8-13)16(19)18-15(11-12-22-3)17(20)21-2
InchiKey: SJJIHHULPKXKSB-UHFFFAOYSA-N
Formula: C17H25NO3S
SMILES: CCCCc1ccc(C(=O)NC(CCSC)C(=O)OC)cc1
Mol. weight [g/mol]: 323.45

Physical Properties

Property code	Value	Unit	Source
gf	-47.73	kJ/mol	Joback Method
hf	-436.47	kJ/mol	Joback Method
hfus	43.53	kJ/mol	Joback Method
hvap	85.14	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.054		Crippen Method
mcvol	261.970	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	868.69	K	Joback Method
tc	1087.32	K	Joback Method
tf	514.44	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.43	J/mol×K	868.69	Joback Method
cpg	804.45	J/mol×K	905.13	Joback Method
cpg	817.26	J/mol×K	941.57	Joback Method
cpg	828.90	J/mol×K	978.00	Joback Method
cpg	839.39	J/mol×K	1014.44	Joback Method
cpg	848.76	J/mol×K	1050.88	Joback Method
cpg	857.05	J/mol×K	1087.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299696&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