L-Methionine, N-(2-chlorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H16ClNO3S/c1-18-13(17)11(7-8-19-2)15-12(16)9-5-3-4-6-10(9)14/h3-6,11

InchiKey: VTGMWNUUHTXXLY-UHFFFAOYSA-N

Formula: C13H16ClNO3S

SMILES: COC(=O)C(CCSC)NC(=O)c1ccccc1Cl

Mol. weight [g/mol]: 301.79

Physical Properties

Property code	Value	Unit	Source
hfus	37.37	kJ/mol	Joback Method
logp	2.364		Crippen Method
mcvol	217.850	ml/mol	McGowan Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	623.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.83	J/mol×K	814.60	Joback Method
cpg	601.74	J/mol×K	853.08	Joback Method
cpg	612.54	J/mol×K	891.56	Joback Method
cpg	622.27	J/mol×K	930.04	Joback Method
cpg	630.95	J/mol×K	968.51	Joback Method
cpg	638.58	J/mol×K	1006.99	Joback Method
cpg	645.21	J/mol×K	1045.47	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299590&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature