L-Phenylalanine, N-(4-bromobenzoyl)-, methyl ester

Inchi: InChI=1S/C17H16BrNO3/c1-22-17(21)15(11-12-5-3-2-4-6-12)19-16(20)13-7-9-14(18)10-

InchiKey: VQRCQNDQAWEMMF-UHFFFAOYSA-N

Formula: C17H16BrNO3

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1ccc(Br)cc1

Mol. weight [g/mol]: 362.22

Physical Properties

Property code	Value	Unit	Source
hfus	38.73	kJ/mol	Joback Method
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-4.49		Cheméo Relay (1.0)
logp	2.963		Crippen Method
mcvol	239.360	ml/mol	McGowan Method
tb	664.14	K	Cheméo Relay (1.0)
tf	371.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.38	J/mol×K	892.75	Joback Method
cpg	682.97	J/mol×K	933.72	Joback Method
cpg	693.41	J/mol×K	974.68	Joback Method
cpg	702.78	J/mol×K	1015.65	Joback Method
cpg	711.14	J/mol×K	1056.61	Joback Method
cpg	718.59	J/mol×K	1097.58	Joback Method
cpg	725.20	J/mol×K	1138.54	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=U299618&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point