Glycine, N-(4-bromobenzoyl)-, methyl ester

Inchi: InChI=1S/C10H10BrNO3/c1-15-9(13)6-12-10(14)7-2-4-8(11)5-3-7/h2-5H,6H2,1H3,(H,12,
InchiKey: BFHPUFUZMOHHQO-UHFFFAOYSA-N
Formula: C10H10BrNO3
SMILES: COC(=O)CNC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 272.10

Physical Properties

Property code	Value	Unit	Source
gf	-123.03	kJ/mol	Joback Method
hf	-302.25	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.352		Crippen Method
mcvol	164.490	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	706.35	K	Joback Method
tc	937.99	K	Joback Method
tf	475.95	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.72	J/mol×K	706.35	Joback Method
cpg	405.35	J/mol×K	744.96	Joback Method
cpg	415.16	J/mol×K	783.56	Joback Method
cpg	424.17	J/mol×K	822.17	Joback Method
cpg	432.41	J/mol×K	860.77	Joback Method
cpg	439.91	J/mol×K	899.38	Joback Method
cpg	446.70	J/mol×K	937.99	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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