3-Bromobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H9BrO2/c1-3-8(2)14-11(13)9-5-4-6-10(12)7-9/h1,4-8H,2H3
InchiKey: MYMIMMHESYRMIQ-UHFFFAOYSA-N
Formula: C11H9BrO2
SMILES: C#CC(C)OC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 253.09

Physical Properties

Property code	Value	Unit	Source
gf	145.55	kJ/mol	Joback Method
hf	22.84	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	58.08	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	2.628		Crippen Method
mcvol	158.430	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	614.87	K	Joback Method
tc	858.99	K	Joback Method
tf	416.60	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.42	J/mol×K	614.87	Joback Method
cpg	355.28	J/mol×K	655.56	Joback Method
cpg	366.25	J/mol×K	696.24	Joback Method
cpg	376.39	J/mol×K	736.93	Joback Method
cpg	385.74	J/mol×K	777.61	Joback Method
cpg	394.33	J/mol×K	818.30	Joback Method
cpg	402.22	J/mol×K	858.99	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=U299139&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