4-Bromobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C12H9BrO2/c1-2-3-4-9-15-12(14)10-5-7-11(13)8-6-10/h1,3-8H,9H2
InchiKey: CPXXHMQKYYUPHF-UHFFFAOYSA-N
Formula: C12H9BrO2
SMILES: C#CC=CCOC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 265.10

Physical Properties

Property code	Value	Unit	Source
gf	236.63	kJ/mol	Joback Method
hf	124.70	kJ/mol	Joback Method
hfus	31.74	kJ/mol	Joback Method
hvap	60.65	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.795		Crippen Method
mcvol	168.220	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	642.35	K	Joback Method
tc	886.45	K	Joback Method
tf	437.79	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.33	J/mol×K	642.35	Joback Method
cpg	379.95	J/mol×K	683.03	Joback Method
cpg	390.68	J/mol×K	723.72	Joback Method
cpg	400.58	J/mol×K	764.40	Joback Method
cpg	409.73	J/mol×K	805.08	Joback Method
cpg	418.19	J/mol×K	845.77	Joback Method
cpg	426.02	J/mol×K	886.45	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U299245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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