4-Bromobutanoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C8H11BrO2/c1-3-7(2)11-8(10)5-4-6-9/h1,7H,4-6H2,2H3
InchiKey: VMCJSLLRIQSERH-UHFFFAOYSA-N
Formula: C8H11BrO2
SMILES: C#CC(C)OC(=O)CCCBr
Mol. weight [g/mol]: 219.08

Physical Properties

Property code	Value	Unit	Source
gf	17.51	kJ/mol	Joback Method
hf	-140.30	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.726		Crippen Method
mcvol	139.920	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1208.00		NIST Webbook
tb	514.57	K	Joback Method
tc	721.90	K	Joback Method
tf	343.85	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.81	J/mol×K	514.57	Joback Method
cpg	296.50	J/mol×K	549.12	Joback Method
cpg	306.64	J/mol×K	583.68	Joback Method
cpg	316.23	J/mol×K	618.23	Joback Method
cpg	325.31	J/mol×K	652.79	Joback Method
cpg	333.88	J/mol×K	687.34	Joback Method
cpg	341.96	J/mol×K	721.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299275&Units=SI

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