5-Bromovaleric acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C9H13BrO2/c1-3-8(2)12-9(11)6-4-5-7-10/h1,8H,4-7H2,2H3
InchiKey: QQDZXNCLKIJSHT-UHFFFAOYSA-N
Formula: C9H13BrO2
SMILES: C#CC(C)OC(=O)CCCCBr
Mol. weight [g/mol]: 233.10

Physical Properties

Property code	Value	Unit	Source
gf	25.93	kJ/mol	Joback Method
hf	-160.94	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.116		Crippen Method
mcvol	154.010	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1368.90		NIST Webbook
tb	537.45	K	Joback Method
tc	741.69	K	Joback Method
tf	355.12	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.24	J/mol×K	537.45	Joback Method
cpg	340.96	J/mol×K	571.49	Joback Method
cpg	352.08	J/mol×K	605.53	Joback Method
cpg	362.61	J/mol×K	639.57	Joback Method
cpg	372.57	J/mol×K	673.61	Joback Method
cpg	381.98	J/mol×K	707.65	Joback Method
cpg	390.86	J/mol×K	741.69	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=U292562&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

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