6-Bromohexanoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C10H15BrO2/c1-3-9(2)13-10(12)7-5-4-6-8-11/h1,9H,4-8H2,2H3
InchiKey: XLDQEPUOOPFDOQ-UHFFFAOYSA-N
Formula: C10H15BrO2
SMILES: C#CC(C)OC(=O)CCCCCBr
Mol. weight [g/mol]: 247.13

Physical Properties

Property code	Value	Unit	Source
gf	34.35	kJ/mol	Joback Method
hf	-181.58	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.507		Crippen Method
mcvol	168.100	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
tb	560.33	K	Joback Method
tc	761.57	K	Joback Method
tf	366.39	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.52	J/mol×K	560.33	Joback Method
cpg	387.15	J/mol×K	593.87	Joback Method
cpg	399.13	J/mol×K	627.41	Joback Method
cpg	410.48	J/mol×K	660.95	Joback Method
cpg	421.22	J/mol×K	694.49	Joback Method
cpg	431.37	J/mol×K	728.03	Joback Method
cpg	440.95	J/mol×K	761.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299286&Units=SI
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

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