4-Bromobutanoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C10H15BrO2/c1-3-6-9(4-2)13-10(12)7-5-8-11/h9H,4-5,7-8H2,1-2H3
InchiKey: FFPLKCIMJWWPHZ-UHFFFAOYSA-N
Formula: C10H15BrO2
SMILES: CC#CC(CC)OC(=O)CCCBr
Mol. weight [g/mol]: 247.13

Physical Properties

Property code	Value	Unit	Source
gf	14.08	kJ/mol	Joback Method
hf	-201.18	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.507		Crippen Method
mcvol	168.100	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	579.21	K	Joback Method
tc	790.63	K	Joback Method
tf	425.52	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.02	J/mol×K	579.21	Joback Method
cpg	388.13	J/mol×K	614.45	Joback Method
cpg	400.58	J/mol×K	649.68	Joback Method
cpg	412.37	J/mol×K	684.92	Joback Method
cpg	423.53	J/mol×K	720.16	Joback Method
cpg	434.07	J/mol×K	755.40	Joback Method
cpg	443.99	J/mol×K	790.63	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=U299278&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