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

Inchi: InChI=1S/C9H11BrO2/c1-2-3-4-8-12-9(11)6-5-7-10/h1,3-4H,5-8H2
InchiKey: DBHFYGRAUDTJAT-UHFFFAOYSA-N
Formula: C9H11BrO2
SMILES: C#CC=CCOC(=O)CCCBr
Mol. weight [g/mol]: 231.09

Physical Properties

Property code	Value	Unit	Source
gf	108.59	kJ/mol	Joback Method
hf	-38.44	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	51.04	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.894		Crippen Method
mcvol	149.710	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	542.05	K	Joback Method
tc	751.01	K	Joback Method
tf	365.04	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.94	J/mol×K	542.05	Joback Method
cpg	320.76	J/mol×K	576.88	Joback Method
cpg	330.95	J/mol×K	611.70	Joback Method
cpg	340.55	J/mol×K	646.53	Joback Method
cpg	349.58	J/mol×K	681.36	Joback Method
cpg	358.09	J/mol×K	716.19	Joback Method
cpg	366.11	J/mol×K	751.01	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=U299277&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