5-Bromovaleric acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C10H13BrO2/c1-2-3-6-9-13-10(12)7-4-5-8-11/h1,3,6H,4-5,7-9H2/b6-3+
InchiKey: SYYDKPSDGIKBFF-ZZXKWVIFSA-N
Formula: C10H13BrO2
SMILES: C#CC=CCOC(=O)CCCCBr
Mol. weight [g/mol]: 245.11

Physical Properties

Property code	Value	Unit	Source
gf	117.01	kJ/mol	Joback Method
hf	-59.08	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	53.26	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.284		Crippen Method
mcvol	163.800	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1588.90		NIST Webbook
rinpol	1588.90		NIST Webbook
tb	564.93	K	Joback Method
tc	770.65	K	Joback Method
tf	376.31	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.66	J/mol×K	564.93	Joback Method
cpg	366.41	J/mol×K	599.22	Joback Method
cpg	377.49	J/mol×K	633.50	Joback Method
cpg	387.94	J/mol×K	667.79	Joback Method
cpg	397.80	J/mol×K	702.08	Joback Method
cpg	407.09	J/mol×K	736.37	Joback Method
cpg	415.86	J/mol×K	770.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292564&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