6-Bromohexanoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C11H15BrO2/c1-2-3-7-10-14-11(13)8-5-4-6-9-12/h1,3,7H,4-6,8-10H2
InchiKey: SUHVFHMCZHPIPE-UHFFFAOYSA-N
Formula: C11H15BrO2
SMILES: C#CC=CCOC(=O)CCCCCBr
Mol. weight [g/mol]: 259.14

Physical Properties

Property code	Value	Unit	Source
gf	125.43	kJ/mol	Joback Method
hf	-79.72	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	55.49	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.674		Crippen Method
mcvol	177.890	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1634.00		NIST Webbook
tb	587.81	K	Joback Method
tc	790.45	K	Joback Method
tf	387.58	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.13	J/mol×K	587.81	Joback Method
cpg	413.69	J/mol×K	621.58	Joback Method
cpg	425.56	J/mol×K	655.36	Joback Method
cpg	436.76	J/mol×K	689.13	Joback Method
cpg	447.34	J/mol×K	722.91	Joback Method
cpg	457.33	J/mol×K	756.68	Joback Method
cpg	466.77	J/mol×K	790.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299288&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