6-Bromohexanoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C12H19BrO2/c1-3-8-11(4-2)15-12(14)9-6-5-7-10-13/h11H,4-7,9-10H2,1-2H3
InchiKey: JRYXFDQXWHHUQM-UHFFFAOYSA-N
Formula: C12H19BrO2
SMILES: CC#CC(CC)OC(=O)CCCCCBr
Mol. weight [g/mol]: 275.18

Physical Properties

Property code	Value	Unit	Source
gf	30.92	kJ/mol	Joback Method
hf	-242.46	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.287		Crippen Method
mcvol	196.280	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1663.00		NIST Webbook
tb	624.97	K	Joback Method
tc	829.86	K	Joback Method
tf	448.06	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.16	J/mol×K	624.97	Joback Method
cpg	486.76	J/mol×K	659.12	Joback Method
cpg	500.61	J/mol×K	693.27	Joback Method
cpg	513.73	J/mol×K	727.42	Joback Method
cpg	526.14	J/mol×K	761.57	Joback Method
cpg	537.84	J/mol×K	795.71	Joback Method
cpg	548.88	J/mol×K	829.86	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=U299289&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