6-Bromohexanoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C15H25BrO2/c1-4-5-9-14(12-13(2)3)18-15(17)10-7-6-8-11-16/h13-14H,4,6-8,1

InchiKey: VLUJDNGBNNOXGI-UHFFFAOYSA-N

Formula: C15H25BrO2

SMILES: CCC#CC(CC(C)C)OC(=O)CCCCCBr

Mol. weight [g/mol]: 317.26

Physical Properties

Property code	Value	Unit	Source
gf	53.74	kJ/mol	Joback Method
hf	-309.66	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	65.95	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.313		Crippen Method
mcvol	238.550	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1856.00		NIST Webbook
tb	693.17	K	Joback Method
tc	893.72	K	Joback Method
tf	466.87	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.59	J/mol×K	693.17	Joback Method
cpg	646.05	J/mol×K	726.60	Joback Method
cpg	661.62	J/mol×K	760.02	Joback Method
cpg	676.33	J/mol×K	793.45	Joback Method
cpg	690.21	J/mol×K	826.87	Joback Method
cpg	703.28	J/mol×K	860.30	Joback Method
cpg	715.57	J/mol×K	893.72	Joback Method

Sources

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=U299291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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