4-Bromobutanoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C14H21BrO2/c1-11(2)7-8-13(10-12(3)4)17-14(16)6-5-9-15/h12-13H,1,5-6,9-10

InchiKey: BHOIDGBQHUREKR-UHFFFAOYSA-N

Formula: C14H21BrO2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)CCCBr

Mol. weight [g/mol]: 301.22

Physical Properties

Property code	Value	Unit	Source
gf	124.61	kJ/mol	Joback Method
hf	-173.38	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.699		Crippen Method
mcvol	220.160	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	666.85	K	Joback Method
tc	876.54	K	Joback Method
tf	439.88	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.62	J/mol×K	666.85	Joback Method
cpg	568.28	J/mol×K	701.80	Joback Method
cpg	583.07	J/mol×K	736.75	Joback Method
cpg	597.00	J/mol×K	771.69	Joback Method
cpg	610.12	J/mol×K	806.64	Joback Method
cpg	622.46	J/mol×K	841.59	Joback Method
cpg	634.03	J/mol×K	876.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299281&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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