4-Bromobutanoic acid, 2-methyl-5-yn-4-yl ester

Inchi: InChI=1S/C13H21BrO2/c1-4-5-7-12(10-11(2)3)16-13(15)8-6-9-14/h11-12H,4,6,8-10H2,1-

InchiKey: NZLLUAVRDDSYOA-UHFFFAOYSA-N

Formula: C13H21BrO2

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

Mol. weight [g/mol]: 289.21

Physical Properties

Property code	Value	Unit	Source
gf	36.90	kJ/mol	Joback Method
hf	-268.38	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.533		Crippen Method
mcvol	210.370	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1638.00		NIST Webbook
tb	647.41	K	Joback Method
tc	853.18	K	Joback Method
tf	444.33	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.54	J/mol×K	647.41	Joback Method
cpg	539.06	J/mol×K	681.70	Joback Method
cpg	553.75	J/mol×K	716.00	Joback Method
cpg	567.64	J/mol×K	750.29	Joback Method
cpg	580.74	J/mol×K	784.59	Joback Method
cpg	593.09	J/mol×K	818.88	Joback Method
cpg	604.69	J/mol×K	853.18	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=U299280&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