4-Bromobutanoic acid, 2,6-dimethylnon-1-en-3--yn-5-yl ester

Inchi: InChI=1S/C15H23BrO2/c1-5-7-13(4)14(10-9-12(2)3)18-15(17)8-6-11-16/h13-14H,2,5-8,1

InchiKey: CHLWIZVUJPTXCY-UHFFFAOYSA-N

Formula: C15H23BrO2

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

Mol. weight [g/mol]: 315.25

Physical Properties

Property code	Value	Unit	Source
gf	133.03	kJ/mol	Joback Method
hf	-194.02	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.089		Crippen Method
mcvol	234.250	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	689.73	K	Joback Method
tc	896.49	K	Joback Method
tf	451.15	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.62	J/mol×K	689.73	Joback Method
cpg	621.73	J/mol×K	724.19	Joback Method
cpg	636.95	J/mol×K	758.65	Joback Method
cpg	651.29	J/mol×K	793.11	Joback Method
cpg	664.80	J/mol×K	827.57	Joback Method
cpg	677.50	J/mol×K	862.03	Joback Method
cpg	689.43	J/mol×K	896.49	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=U299282&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